

# **A User's Guide for the Prediction of Post-Mining Groundwater Chemistry from Overburden Characteristics**



**Heritage Fund**



LAND CONSERVATION AND  
RECLAMATION COUNCIL  
Reclamation Research  
Technical Advisory Committee

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Regulating surface disturbances in Alberta is the responsibility of the Land Conservation and Reclamation Council. The Council executive consists of a Chairman from Alberta Environment and two Deputy Chairmen from Alberta Forestry, Lands and Wildlife. The Council oversees a reclamation research program, established in 1978, to identify the most efficient methods for achieving acceptable reclamation in the province. Funding for the research program is provided by Alberta's Heritage Savings Trust Fund, Land Reclamation Program.

To assist with the development and administration of the research program, the Council appointed the inter-departmental Reclamation Research Technical Advisory Committee (RRTAC). The Committee consists of eight members representing the Alberta Departments of Agriculture, Energy, Forestry, Lands and Wildlife, and Environment, and the Alberta Research Council. The Committee updates research priorities, reviews research proposals, organizes workshops, and otherwise acts as the coordinating body for reclamation research in Alberta.

Additional information on the Reclamation Research Program may be obtained by contacting:

**Chris Powter, Chairman**  
**Reclamation Research Technical Advisory Committee**  
**Alberta Environment**  
**3rd Floor, Oxbridge Place**  
**9820 - 106 Street**  
**Edmonton, Alberta T5K 2J6**  
**(403) 427-4147**

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**A USER'S GUIDE  
FOR THE PREDICTION  
OF POST-MINING GROUNDWATER CHEMISTRY  
FROM OVERBURDEN CHARACTERISTICS**

by

M.R. TRUDELL

D.B. CHEEL

Terrain Sciences Department

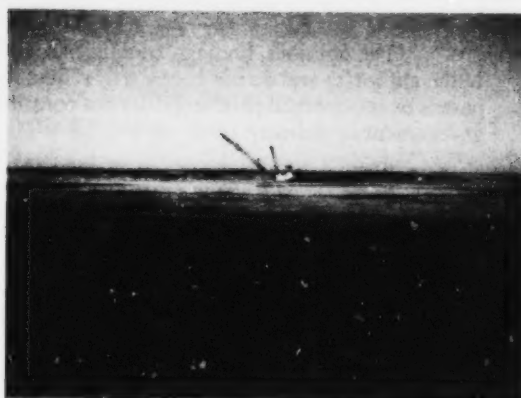
Alberta Research Council

Prepared for

The Plains Coal Reclamation Research Program  
ALBERTA LAND CONSERVATION AND RECLAMATION COUNCIL  
(Reclamation Research Technical Advisory Committee)



## Plains Coal Reclamation Research Program



**Members:** Chris Powter (Chairman) - Alberta Environment; Lilli Chevrier (Secretary) - Alberta Environment; Yeh Moon Chae - Alberta Environment; John Dormaar - Agriculture Canada; Katherine Gizikoff - Manalta Coal Ltd.; John Hastie - TransAlta Utilities Corporation; Richard Johnson - Alberta Environmental Centre; Jivan Kayande - Alberta Power Limited; Chong Ko - Alberta Environment; Dermot Lane - Fording Coal Ltd.; Bob Logan - Luscar Ltd.; Leon Marciak - Alberta Agriculture.

## **DISCLAIMER**

This report is intended to provide government and industry staff with up-to-date technical information to assist in the preparation and review of Development and Reclamation Approvals, and development of guidelines and operating procedures. This report is also available to the public so that interested individuals similarly have access to the most current information on land reclamation topics.

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## PREFACE

This volume is part of a series of reports that presents the findings of the Plains Hydrology and Reclamation Project (PHRP), an interdisciplinary study that focuses primarily on hydrologic aspects of reclamation of surface coal mines in the Plains of Alberta. This research has been conducted by the Alberta Research Council, as part of the Alberta Government's Reclamation Research Program. The program is managed by the Land Conservation and Reclamation Council and is supported by the Alberta Heritage Savings Trust Fund, Land Reclamation Program.

The focus of the PHRP is to develop a predictive framework that will permit projection of success for reclamation and impact of mining on water resources on a long-term basis. The predictive framework is based on an understanding of processes acting within the landscape so that, in the future, mine sites that are not totally analogous to those that have been studied can be evaluated as well.

The project involves a holistic approach to reclamation by integration of studies of geology, hydrogeology, and soils, not only in the proposed mining area, but also in the adjoining unmined areas. This approach permits the assessment of impacts and of long-term performance, not only in reclaimed areas, but also in the surrounding area.

The research of the PHRP has been directed toward the following two major objectives and eight subobjectives:

### Objective A

To evaluate the potential for reclamation of lands to be surface mined. The focus is on features of the landscape that make it productive in a broad sense not restricted to revegetation. This objective was organized into five subobjectives.

1. To assess and evaluate the potential for long-term degradation of reclaimed soils through salt buildup.

2. To assess and evaluate the effectiveness of topographic modification and selective placement of materials to mitigate deleterious impacts on chemical quality of groundwater.
3. To assess the availability of water supply in or beneath cast overburden to support post-mining land use, including both quantity and quality considerations.
4. To evaluate the productivity potential (capability) of post-mining landscapes and the significance of changes in capability as a result of mining.
5. To assess and evaluate limitations to post-mining land use posed by physical instability of cast overburden.

#### Objective B

To evaluate the long-term impact of mining and reclamation on water quantity and quality. This objective was organized into three subobjectives.

1. To assess and evaluate the long-term alteration of quality of groundwater in cast overburden and surface water fed from mine spoil as a result of the generation of weathering products.
2. To assess and evaluate infiltration, groundwater recharge, and groundwater-surface water interactions within cast overburden.
3. To characterize the groundwater chemistry generated within cast overburden.

Studies directed at these objectives began in 1979 at the Battle River site in east-central Alberta. Work began in 1982 at a second study area at Highvale Mine south of Lake Wabamun.

This report, together with its companion report "Prediction of Post-Mining Groundwater Chemistry from Overburden Characteristics" (Trudell et al., in press) addresses Subobjective A-1, focusing on the generation of salinity in spoil groundwater. Saline spoil

groundwater is a contributing factor to the development of salinization in reclaimed landscapes, particularly in shallow water-table settings.

This report provides the detailed procedure and methodology that is required to produce a prediction of post-mining groundwater chemistry based on the soluble salt characteristics of overburden materials. The contribution from weatherable salts has been found to be negligible relative to the large reservoir of pre-existing soluble salts, and therefore only pre-existing soluble salts are considered by the predictive procedure. A fundamental component of the procedure for predicting the chemistry of spoil groundwater is the geochemical model 'PHREEQE', developed by the U.S. Geological Survey (USGS) (Parkhurst et al. 1980). This public domain software is available from the USGS. Although written for mainframe computer systems, modified versions have been adapted by individual users to allow running the program on personal computers. In any case, access to this model is required in order to carry out the prediction of spoil groundwater chemistry by the procedure described in this report.

ABSTRACT

This report describes a method by which it is possible to predict the chemical composition and salinity of groundwater in mine spoil strictly on the basis of premining overburden and groundwater characteristics. The predictive model relies on the use of an aqueous geochemical model (PHREEQE) to allow consideration of partial pressures of carbon dioxide, ion exchange, and mineral dissolution/precipitation in the simulated spoil groundwater.

The basis of the predictive model is the characterization of overburden salt-yielding properties determined by leaching tests.

There are five steps involved in the simulation of post-mining groundwater chemistry: (1) characterization of overburden salt-yielding properties; (2) construction of hypothetical spoil material based on the overburden salt characteristics; (3) conceptual saturation of the hypothetical spoil with water, allowing the dissolution of the salts; (4) definition of geochemical conditions in the spoil; (5) application of the USGS geochemical model PHREEQE to control and manipulate geochemical parameters. With this program, the chemical composition of solutions in equilibrium with both solid and gaseous phases can be calculated. In addition, the reservoir of soluble salt remaining after one pore-volume of flushing can be determined.

### ACKNOWLEDGEMENTS

The Plains Hydrology and Reclamation Project was sponsored by the Reclamation Research Technical Advisory Committee of the Alberta Land Conservation and Reclamation Council, with financial support from the Alberta Heritage Savings Trust Fund, Land Reclamation Program, Alberta Power Limited, Luscar Ltd., Manalta Coal Ltd., and TransAlta Utilities Corporation, for providing both available data and access to lands for the research work are gratefully acknowledged.

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1.

## INTRODUCTION

This user's guide is a companion to the report "Prediction of Post-Mining Groundwater Chemistry from Overburden Characteristics" (Trudell, et al., in press). The purpose of this manual is to document the procedure by which predictions of post-mining groundwater chemistry were made in the above report. In addition, this manual will provide the reader with information on the procedure for predicting groundwater chemistry so that simulations can be carried out by others.

There is a significant overlap between this manual and its companion report. This overlap is required so that each document forms a coherent, stand-alone publication. In most cases, the common sections on modelling methodology are more general in this manual than in the report.

Included in this manual is a completely documented example prediction, worked through in detail from leach-test extract to final predicted groundwater chemistry. It is hoped that this example will act to clarify any ambiguities within the text.

As well as the discussion of the methodology and worked-through example, this document includes an appendix summarizing the geochemical model PHREEQE.

## 2. SUMMARY OF MODELLING METHODOLOGY

There are five steps involved in the simulation of post-mining groundwater chemistry: (1) characterization of overburden salt-yielding properties; (2) construction of hypothetical spoil material based on the overburden salt characteristics; (3) conceptual saturation of the hypothetical spoil with water, allowing the dissolution of the salts; (4) definition of geochemical conditions in the spoil; (5) application of the geochemical model PHREEQE to control and manipulate geochemical parameters. PHREEQE is a computer program developed by the U.S. Geological Survey (USGS) that can be used to calculate pH, redox potential, and mass transfer between solid, solution, and gaseous phases during a reaction (Parkhurst et al. 1980). With this program the chemical composition of solutions in equilibrium with both solid and gaseous phases can be calculated.

Figure 1 is a flow-chart representation of the simulation procedure that is described in the following sections. A simple outline of the procedure is as follows:

1. Characterize the salt-yielding properties of "typical" overburden at site in question:
  - a. Determine salt-yield of representative overburden samples using an aqueous extract technique (saturated paste or 10:1 water to sediment). Convert the concentration of each ion to salt-yield in g/kg using water and solid amounts from the extraction procedure. Calculate the yield of each ion for each sample.
  - b. Group data by meaningful stratigraphic subdivisions. For example, in Alberta study sites only two overburden units are meaningful: drift and bedrock.
  - c. Summarize the salt-yielding characteristics for each stratigraphically meaningful unit. A variety of options are available including mean-standard

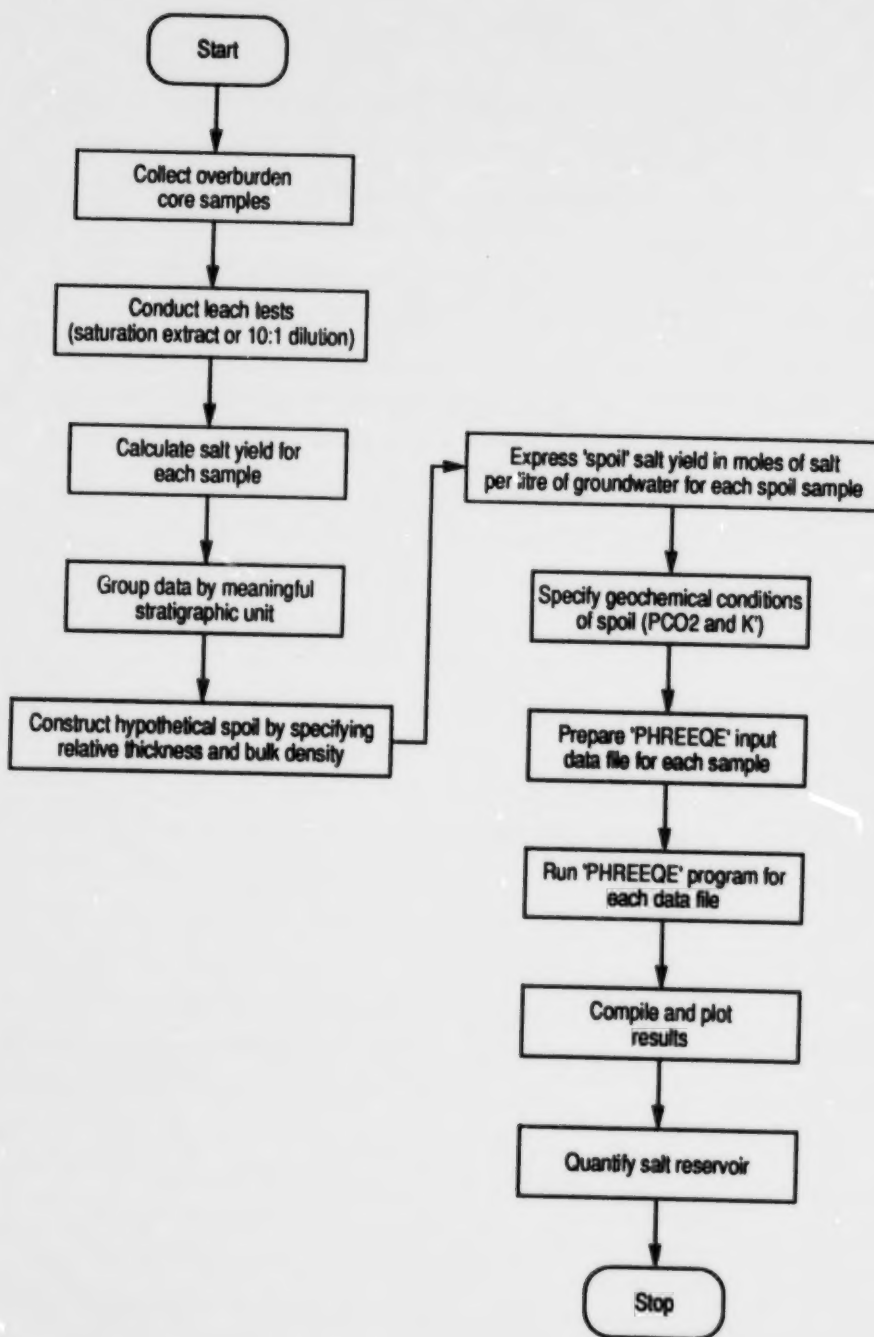


Figure 1. Flow chart of procedure for simulation/prediction of spoil groundwater chemistry.

deviation methods and cumulative frequency-based methods. The method used would depend partially on the number of samples used to characterize the unit.

2. Construct hypothetical spoil material from the overburden salt-yield data:
  - a. Determine the relative contribution from each stratigraphic unit to the total spoil salt by determining the relative thickness of each unit in the overburden under consideration.
  - b. Calculate the soluble salt content of the hypothetical spoil material from the thickness-weighted average of each overburden unit's salt-yield.
3. Saturate (conceptually) the hypothetical spoil with water, allowing the dissolution of the salts.
  - a. At an assumed saturated porosity of 30%, each litre of water is in contact with 6.2 kg of spoil material. Alternately, calculate mass of spoil per litre of water at the expected spoil bulk density.
  - b. Express the salt-yield data for each sample as moles of each ion per litre of water. This is then written as a soluble salt "reaction mineral" representing the salt in the spoil.
  - c. The salt yielded by the mass of spoil from 3.a. is considered to dissolve in the pore water.
4. Define the geochemical conditions in the spoil.
  - a. Partial pressure of  $\text{CO}_2$  ( $P_{\text{CO}_2}$ ) can be estimated from (i) existing data, or (ii) from the  $P_{\text{CO}_2}$  values calculated by a geochemical speciation (e.g., PHREEQE calculation) from chemical analyses of overburden groundwater samples.

- b. Ion exchange can be estimated by determining modified selectivity coefficient values from geochemical speciation of chemical analyses of overburden groundwater samples.
- 5. Apply the aqueous geochemistry model PHREEQE.
  - a. The mineral saturation/solubility constraints for commonly occurring sparingly soluble minerals, especially calcite, dolomite, and gypsum are applied to the system using the equilibrium model PHREEQE.
  - b. The hypothetical solution is generally supersaturated with respect to calcite and dolomite, and sometimes gypsum; these minerals are allowed to precipitate to saturation, taking into account the geochemical conditions of the system.
  - c. Once equilibrium is attained, the model generates output, which indicates the chemical composition of the water and the amount of each mineral that remains in solid form.

### 3. PROCEDURE FOR PREDICTING POST-MINING GROUNDWATER CHEMISTRY FROM OVERBURDEN CHARACTERISTICS

#### 3.1 OVERBURDEN CHARACTERIZATION FROM LEACH TESTS

Overburden samples are collected from a number of undisturbed sites by means of rotary coring and/or Shelby tube sampling. Sub-samples are taken from selected lithologic intervals within each core hole, for leach test analysis. Standard saturated paste extract (SE) analyses are one type of leach test that can be used to determine the soluble salt content of the overburden. In relatively saline overburden materials, a 10:1 (water to sediment) leach test is preferred. In this test, 50 mL of water is added to a 5-gram sample, agitated for approximately one-half hour, then centrifuged and the supernatant fluid collected. Chemical analysis of dissolved ions is carried out on the leach test extract regardless of the type of test carried out.

In general, the characterization of overburden salt-yielding characteristics by saturated paste extract tests produces the best prediction of post-mining groundwater chemistry.

#### 3.2 SALT-YIELD CALCULATIONS

It is necessary to convert the ionic concentrations (in mg/L) that are the product of the leach test analyses into a mass of salt per mass of overburden material (i.e., grams of salt per kg of overburden). For saturation extract analyses, this is accomplished by the relationship,

$$Y_i (\text{g/kg}) = C_i (\text{g/m}^3) \times S (\text{kg H}_2\text{O/kg sample}) / 1000 \text{ kg/m}^3 \quad (1)$$

where  $Y_i$  = yield of constituent  $i$  (g/kg)

$C_i$  = concentration of constituent  $i$  in the extract  
(mg/L = g/m<sup>3</sup>)

and  $S$  = saturation percent, expressed as a decimal fraction.

For the 10:1 (water:sediment) leach test samples, the calculation of salt-yield is accomplished by simply expressing the mass of constituent  $i$  in the extract in terms of the correct units, for example,

$$Y_i(\text{g/kg}) = C_i(\text{g/m}^3) \times V(\text{m}^3)/M(\text{kg}) \quad (2)$$

where  $V$  = volume of water used in the test, in  $\text{m}^3$ , and  
 $M$  = mass of sample used in the test, in kg.

The yield of each ionic constituent is determined in this fashion and the sum of the yields for all ionic constituents of a sample is the total salt-yield, or yield of total dissolved solids (TDS) for the sample.

### 3.3 DATA GROUPING APPROACHES

The leach test data from overburden core samples must be grouped in some manner that approximates the distribution of materials, and more importantly, salts that will ultimately make up the spoil. The leach test samples are initially segregated by stratigraphic (geologic) unit. For example, in the plains region of Alberta, two meaningful stratigraphic subdivisions of overburden materials were identified in terms of salt-yield properties: (1) glacial drift; (2) bedrock overburden (Maslowski Schutze 1986; Trudell et al. 1983, in press).

Four approaches to the grouping of overburden salt-yield data for each overburden unit are suggested: (1) for each corehole, the mean and standard deviation salt-yield is calculated ('Mean Corehole Approach'); (2) for all available samples, the mean and standard deviation salt-yield is calculated ('Mean and Standard Deviation' grouping); (3) from all available samples, sub-groups corresponding to percentiles of EC cumulative frequency distribution are selected ('EC Percentile-based Approach'); (4) from all available samples, sub-groups corresponding to sulfate cumulative frequency

distribution percentiles are selected ('Sulfate Percentile-based Approach'). These approaches are discussed below.

### 3.3.1 Mean Corehole Approach

Core samples of overburden are collected on a site by site basis. In the 'Mean Corehole' approach, the salt-yield characteristics of mine spoil are estimated from the mean salt-yield characteristics of the overburden materials based on individual coreholes. Soluble salt data from each of the coreholes sampled are used as the basis for simulations of spoil groundwater chemistry. In addition to the mean values of each overburden unit, the mean  $\pm 1$  SD salt-yields can be used to represent a possible range of spoil materials.

### 3.3.2 Mean and Standard Deviation Groupings

From all the available analyses of each overburden unit, a mean and standard deviation (SD) for the salt-yield are calculated. To cover the range of possible spoil materials, the mean salt-yield and the mean  $\pm$  standard deviation(s) are used.

### 3.3.3 Percentile-Based Data Groupings

Percentile-based approaches rely on two of the principal characteristics of the leach test extracts - EC and sulfate concentration - as the basis for grouping data. More specifically, the cumulative frequency distributions of EC or sulfate in the sample extracts can be used to represent the salt-yield characteristics of the overburden. An example of this type of distribution is shown in Figure 2; the sample selection process is outlined schematically in Figure 3. In order to provide a representation of the range of salinities present in the sample population, small groups of samples are selected, corresponding to the desired percentiles of the cumulative frequency distribution of EC or sulfate. These small groups include all samples within one class size of the percentile.

This method of selecting and grouping data is conducted separately for the analyses from each overburden unit.

As in the previous two methods, hypothetical spoil is produced by combining the cumulative frequency groupings from each overburden unit, weighted by the relative thickness of each unit. Hypothetical spoil material from percentile-based groupings can produce a range of possible spoil materials from low salinity (for example, from the 10 percentile groups), to moderate salinity (from the 50 percentile groups), to high salinity (from the 90 percentile groups).

### 3.3.4 Comparison of Data Grouping Techniques

The four approaches above were evaluated for their suitability for simulating spoil groundwater at Vesta Mine in the Battle River mining area of Alberta. All are capable of simulating the mean spoil groundwater composition and salinity. The principal

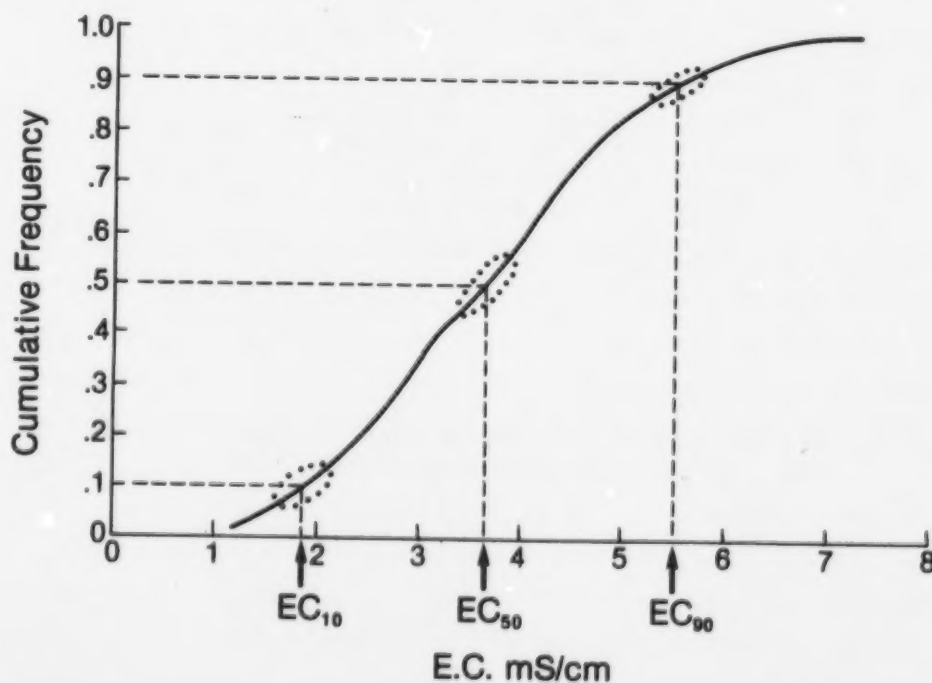


Figure 2. Example of cumulative frequency distribution for electrical conductance (EC) from leach test extracts.

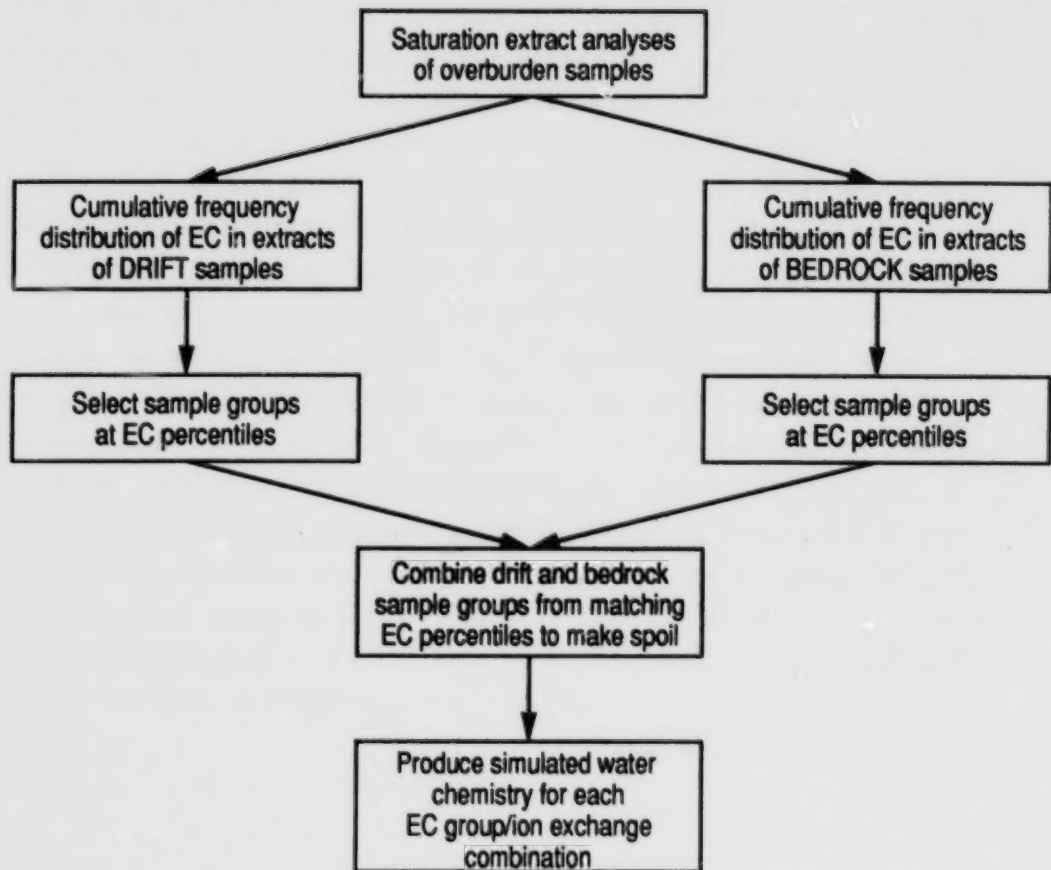


Figure 3. Schematic representation of sample grouping process for simulation of spoil groundwater chemistry.

characteristic differentiating the success of the various approaches is the simulation of not only the mean spoil groundwater chemistry, but also the range of spoil groundwater chemistry.

The sulfate-based percentile approach provided the best overall simulation of the Vesta Mine spoil groundwater chemistry, particularly in terms of representing the variability that is characteristic of the spoil groundwater. The EC-based percentile approach provided the second best overall representation of the spoil groundwater. The corehole mean salt and overall mean and SD approaches both produced good simulations of the mean and high salinity spoil groundwater, but performed less well than the percentile-based approaches in terms of characterizing the full range of spoil groundwater composition and salinity.

For EC-based data grouping, suitable predictions of spoil groundwater chemistry have been obtained for:

1. Ten, 50, and 70 percentile groups of 10:1 dilution test data.
2. Fifty, 70, and 90 percentile groups of SE test data.

For sulfate-based data grouping, acceptable predictions of spoil groundwater chemistry have been obtained for:

1. 10, 50, and 70 percentile groups of 10:1 dilution test data.
2. 50, 70, and 90 percentile groups of SE test data.

There are some cases where simulations from percentile groups other than those listed above matched observed spoil groundwater chemistry; however, the above generalizations provided the best overall agreement for both Vesta and Highvale settings.

### 3.4 CONSTRUCTING HYPOTHETICAL SPOIL

The salt-yield characteristics of the stratigraphic units making up the overburden that becomes the spoil material are combined to produce a 'hypothetical spoil' to be used for simulating spoil groundwater chemistry. The relative proportions of each overburden unit that make up the spoil are accommodated by weighting the

components by a factor that corresponds to their relative thickness. For example, in a mine where the overburden is one-third drift and two-thirds bedrock, the weighting factors would be 0.33 drift:0.67 bedrock. The weighting factors are then applied to the salt-yields from each overburden unit in order to approximate the salt-yield capability of the hypothetical spoil material.

### 3.5 GEOCHEMICAL CONDITIONS IN RECLAIMED SPOIL

The dissolution of salts in spoil groundwater is subject to the constraints of mineral solubility, especially with respect to calcite, dolomite, and gypsum; partial pressure of carbon dioxide ( $P_{CO_2}$ ), which is typically higher than atmospheric levels, and ion exchange. Mineral solubility limits are well defined in the geochemical literature, based on solubility products ( $K_{sp}$ ), and are easily handled mathematically by aqueous geochemical models such as PHREEQE, described in later sections of this report.

#### 3.5.1 Partial Pressure of $CO_2$

Partial pressures of  $CO_2$  in reclaimed spoil can be dealt with by one of two empirical techniques. The first is based on measured values reported in the literature, the second is calculated from premining groundwater chemistry. In Alberta, the only measurements of actual  $P_{CO_2}$  levels in reclaimed spoil are reported by Wallick (1983). The measurements represent three mines in the two principal coal zones of the province. Vesta and Diplomat Mines are in the Lower Horseshoe Canyon Formation Coal Zone in the Battle River mining area (Figure 4). At Vesta Mine the overburden is composed of mixed drift and bedrock of the Horseshoe Canyon Formation; at Diplomat Mine the overburden is almost entirely glacial drift. Highvale Mine is in the Ardley Coal Zone in the Lake Wabamun mining area (Figure 4) and has overburden that includes glacial drift and bedrock of the Paskapoo Formation. The reported  $P_{CO_2}$  values for these mines are summarized in Table 1. For the purpose of predicting

Table 1. Partial pressure of  $\text{CO}_2$  measured in reclaimed mine spoil - central Alberta (Wallick 1983).

| Mine              | Log $P_{\text{CO}_2}$ (Atmospheres) |       |         |         | Calculated Mean |
|-------------------|-------------------------------------|-------|---------|---------|-----------------|
|                   | Mean                                | SD    | Minimum | Maximum |                 |
| Vesta             | -1.575                              | 0.246 | -2.49   | -1.30   | -2.395          |
| Diplomat          | -1.316                              | 0.669 | -2.80   | -0.64   | -1.991          |
| Highvale (Pit 01) | -1.748                              | 0.698 | -3.70   | -0.86   | -2.148          |

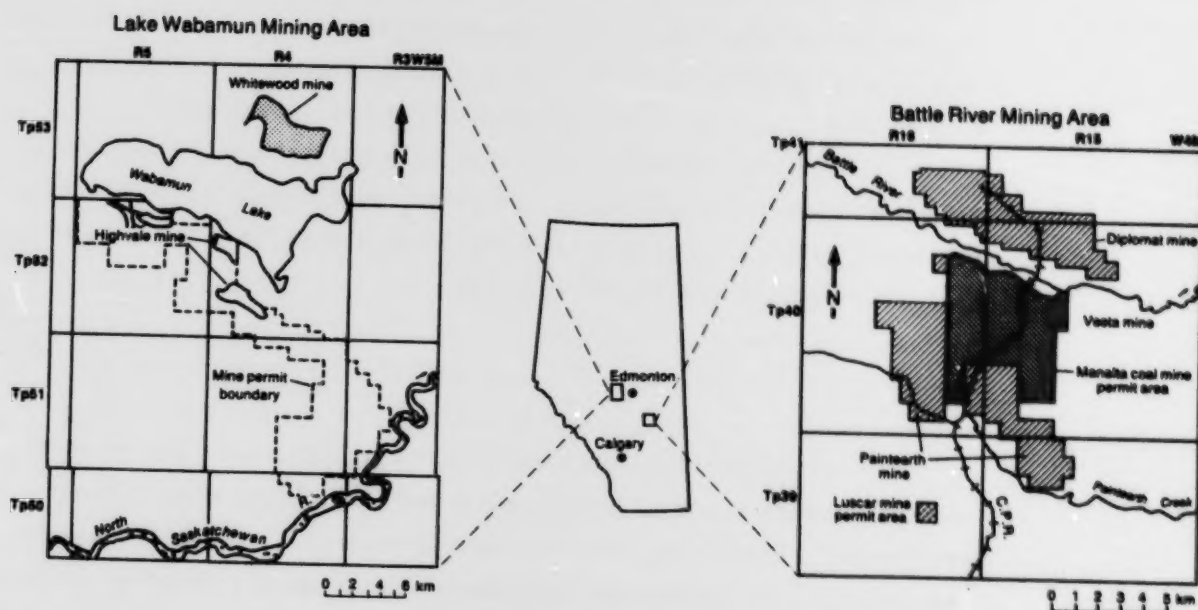


Figure 4. Map showing location of mines in the Battle River mining area and the Lake Wabamun mining area, central Alberta.

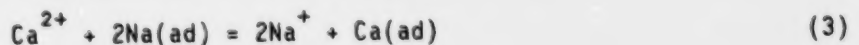
spoil groundwater chemistry, the mean  $P_{CO_2}$  values have been used in most cases.

The second technique for estimating  $P_{CO_2}$  levels in mine spoil is based on calculations of equilibrium  $P_{CO_2}$  levels from groundwater samples from unmined overburden. Aqueous geochemical models such as WATEQF or PHREEQE, in performing a speciation analysis of a groundwater chemistry sample, calculate the  $P_{CO_2}$  at which the sample was in equilibrium. The log mean  $P_{CO_2}$  calculated from the overburden groundwater samples is generally lower than the observed log mean  $P_{CO_2}$  in reclaimed spoil, based on observations at Diplomat, Vesta, and Highvale Mines.

### 3.5.2 Ion Exchange

Ion exchange between free cations in solution, particularly divalent cations such as  $Ca^{2+}$ , and cations adsorbed onto clay particle surfaces (especially monovalent cations such as  $Na^+$ ) is an important process affecting groundwater chemistry in nearly all subsurface environments. In the premining spoil groundwater environment in the Plains setting, ion exchange is particularly significant because of the relatively large amount of fine-grained (i.e., clayey or clay-bearing) sediment in the overburden.

The process of ion exchange in a groundwater system can be viewed as a reversible chemical reaction involving solution and solid (adsorbed) phases. For the exchange of dissolved  $Ca^{2+}$  for adsorbed  $Na^+$ , the reaction can be expressed as,



It is desirable to base projections of spoil ion exchange characteristics on easily measured properties of the premining overburden. Therefore, a simplified version of the traditional selectivity coefficient approach to ion exchange was sought. As a result, the technique of approximating the ion exchange characteristics of a material based on water chemistry as described

by Parkhurst et al. (1980) was adopted. In their analysis, the parameter  $K'$ , which will be referred to in this paper as the modified selectivity coefficient, is defined as,

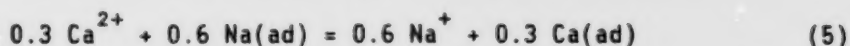
$$K' = [\text{Na}^+]^2 / [\text{Ca}^{2+}] \text{ for Ca-Na Exchange} \quad (4)$$

where square brackets  $[\ ]$  represent activity, and  $K'$  is the modified selectivity coefficient of the  $\text{Na}^+ - \text{Ca}^{2+}$  exchange reaction. This approximation is valid in systems with a large reservoir of exchangeable  $\text{Na}^+$  and  $\text{Ca}^{2+}$  relative to dissolved concentrations. In such a case, the amount of adsorbed  $\text{Na}^+$  and  $\text{Ca}^{2+}$  is approximately constant, and the right side of Equation (4) represents an approximately constant quantity equal to  $K'$ .

As described above, the modified selectivity coefficient ( $K'$ ) is a function of the activity of dissolved  $\text{Na}^+$  and  $\text{Ca}^{2+}$  in groundwater; therefore, it is necessary to have chemical analyses of groundwater from unmined overburden to determine  $K'$  values for the overburden materials. Converting analytical concentrations of  $\text{Ca}^{2+}$  and  $\text{Na}^+$  in groundwater into the thermodynamic activity values required for the determination of  $K'$  is a difficult calculation to accomplish manually, but is readily done with the aid of aqueous geochemical models such as WATEQF or PHREEQE.

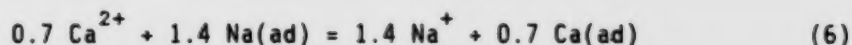
From unmined overburden groundwater analyses, a mean  $K'$  value can be determined for each stratigraphic unit of the overburden material. Because of the very wide range possible for  $K'$  values (several orders of magnitude) it is usually necessary to perform a log transform of the data to normalize it. In order to produce a predicted  $K'$  value for 'spoil' the mean  $K'$  values of the overburden units are combined, based on their relative thickness. It is possible to estimate the spoil  $K'$  value if one assumes that the overall molar contribution from the overburden units is equal to their respective relative thickness. For example, in a case where the overburden consists of two units, drift and bedrock, with

relative thickness of 0.3 and 0.7 respectively, then the ion exchange reaction for the drift can be written as,



for which the  $K'$  value ( $K'_g$ ) is equal to the drift  $K'_{\text{Ca-Na}}^{0.3}$ .

Similarly, for the bedrock contribution, the ion exchange reaction is,



for which the  $K'$  value ( $K'_g$ ) is equal to the bedrock  $K'_{\text{Ca-Na}}^{0.7}$ . Adding reactions (5) and (6) yields the assumed net ion exchange reaction for the spoil, for which the spoil  $K'_g$  value is  $K'_g \times K'_g$ . Alternately, these relationships can be expressed in logarithmic form, that is (for this example),

$$\log K'_g = 0.3 \log K'_{\text{drift}} + 0.7 \log K'_{\text{bedrock}} \quad (7)$$

or in more general terms:

$$\begin{aligned} \log K'_g = & \text{thick}_{\text{unit1}} \log K'_{\text{unit1}} + \\ & \text{thick}_{\text{unit2}} \log K'_{\text{unit2}} + \dots \\ & \text{thick}_{\text{unitn}} \log K'_{\text{unitn}} \end{aligned} \quad (8)$$

where  $\text{thick}$  = relative thickness of each overburden unit.

To calculate an estimated  $K'$  value for the predicted spoil material, Equation (8) is used, substituting the actual relative thicknesses of each of the overburden units making up the spoil.

In the above example, the  $K'$  values used for drift and bedrock were the log-mean values calculated from several groundwater analyses. The range of  $K'$  values observed in overburden materials is taken into consideration by calculating mean  $K' + 2 \text{ SD}$  and mean

$K' - 2$  SD values. As with the mean  $K'$  value, maximum and minimum  $K'$  values are determined from log mean and log SD values. To obtain an estimate of the maximum and minimum  $K'$  values of spoil material, Equation (8) is again used with the weighting factors for relative thickness (as was done above) for the mean spoil  $K'$ .

The procedure for estimating the ion exchange characteristics of spoil described above can be summarized as follows: (1) calculate log mean  $K'$  and log SD values for each overburden unit; (2) calculate a thickness - weighted average of the overburden log mean  $K'$  values, using the relative proportions of each overburden unit with Equation (8), to approximate the mean spoil  $K'$ ; (3) calculate a thickness-weighted average of the overburden log mean  $K' \pm 2$  SD using Equation (8), to approximate the minimum and maximum spoil  $K'$  values.

In addition to  $\text{Ca}^{2+} - \text{Na}^+$  ion exchange, it is possible to have exchange of dissolved  $\text{Mg}^{2+}$  for  $\text{Na}^+$  adsorbed on clay surfaces. In most cases, where a significant proportion of the overburden is bedrock, the amount of soluble  $\text{Mg}^{2+}$  is sufficiently small that  $\text{Mg}^{2+} - \text{Na}^+$  exchange can be neglected. However, in situations where there is a significant proportion of soluble  $\text{Mg}^{2+}$  among the soluble cations, as in the case of mines with drift-dominated overburden,  $\text{Mg}^{2+} - \text{Na}^+$  exchange must be considered in predicting spoil groundwater chemistry. The treatment of  $\text{Mg}^{2+} - \text{Na}^+$  exchange is identical to that of  $\text{Ca}^{2+} - \text{Na}^+$  exchange, and produces a value for  $K'_{\text{Mg}} - N_{\text{Na}}$ . Experience at several mine sites, including both drift and bedrock-dominated overburden, indicates that  $\text{Mg}^{2+} - \text{Na}^+$  exchange should be considered where the available calcium plus magnesium (in moles) in the spoil soluble salt is greater than about 25% of the available  $\text{Na}^+$  (in moles); also the amount of soluble  $\text{Mg}^{2+}$  (in moles) should be about the same magnitude as the amount of soluble  $\text{Ca}^{2+}$ .

The only other consideration in dealing with  $\text{Mg}^{2+} - \text{Na}^+$  exchange relates to numerical problems encountered when fixing both  $K'_{\text{Ca}} - N_{\text{Na}}$  and  $K'_{\text{Mg}} - N_{\text{Na}}$  together with a saturation constraint on the

mineral dolomite. As explained by Parkhurst et al. (1980, pp. 50) this situation exceeds the numerical limits of the model and, therefore, must be avoided. By imposing the above conditions sequentially rather than simultaneously, it is possible to arrive a reasonable approximation for the required simulation.

### 3.6 SATURATION OF SPOIL MATERIAL AND APPLICATION OF THE AQUEOUS GEOCHEMICAL MODEL PHREEQE

In this section, the procedure for applying the USGS computer program PHREEQE to the problem of predicting post-mining groundwater chemistry is described. The objective of this section is to describe the application of PHREEQE in sufficient detail that persons acquainted with the program might undertake a similar analysis, and also to show the kind of calculations the program is able to provide. It is not the purpose of this report to fully describe the program or its input requirements, which are discussed in detail by Parkhurst et al. (1980) in the program User's Manual; however, a brief summary of the model and its input is given in Appendices 6.1 and 6.2.

The purpose of utilizing PHREEQE in the simulation of post-mining groundwater chemistry is to enable the consideration of: (1) mineral solubility limits that may be reached during dissolution of salts from the spoil; (2) the effects of elevated partial pressures of  $\text{CO}_2$  that have been observed in spoil; (3) the effects of ion exchange between species in solution and ions adsorbed onto clay mineral surfaces in the spoil. An additional feature of the program is its ability to quantify the amount of salt that is in excess of mineral solubility limits and, therefore, acts as a reservoir of undissolved salt for dissolution when fresh water enters the spoil after initial resaturation.

Applying PHREEQE to the prediction of spoil groundwater chemistry involves converting the spoil salt-yield data (grams of salt per kg of spoil) into units of moles of salt per litre of water. This can be done using the following formula:

$$\text{Moles/Litre}_i = Y_i (\text{g/kg}) \times M_s (\text{kg/L}) / \text{GFW}_i (\text{g/Mole}) \quad (9)$$

where  $Y_i$  = salt-yield of constituent  $i$ ,  
 $\text{GFW}_i$  = gram formula weight (or atomic weight) of constituent  $i$ ,  
 and  $M_s$  = mass of spoil solids per litre of pore space.  
 $M_s$  is determined from the following density relationship:

$$\rho_b = M_s - \frac{\rho_b}{\rho_s} M_s \quad (10)$$

where  $\rho_b$  = dry bulk density ( $\text{g/cm}^3$ )  
 $\rho_s$  = particle density ( $\text{g/cm}^3$ )

The salt thus defined represents material that is in the solid phase, but is available to dissolve in 1 L of water. As a solid soluble salt it may be viewed as a 'mineral' phase, composed of cationic ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ) and anionic species ( $\text{SO}_4^{2-}$ ,  $\text{HCO}_3^-$ ,  $\text{Cl}^-$ ) which combine in this solid 'mineral' phase to form a single, soluble substance. This soluble substance, which will be referred to as the 'soluble salt mineral', has all of the major ionic species as constituents. The proportion of each of the ionic species in this reaction mineral is determined by the moles of that species available per litre of water.

As an example, consider a spoil material with the following salt-yield characteristics:

0.64 g/kg  $\text{Ca}^{2+}$   
 0.38 g/kg  $\text{Mg}^{2+}$   
 0.74 g/kg  $\text{Na}^+$   
 0.06 g/kg  $\text{K}^+$   
 4.64 g/kg  $\text{SO}_4^{2-}$   
 0.06 g/kg  $\text{Cl}^-$   
 0.98 g/kg  $\text{HCO}_3^-$

Using Equation (9), with  $M_s = 6.2 \text{ kg/L}$  (bulk density =  $1.854 \text{ g/cm}^3$ ), the moles of each constituent per litre of water are determined, that is,

0.10 Mole  $\text{Ca}^{2+}/\text{L}$

0.10 Mole  $\text{Mg}^{2+}/\text{L}$

0.20 Mole  $\text{Na}^+/\text{L}$

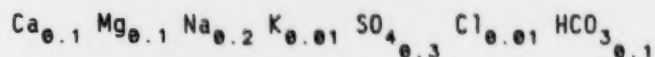
0.01 Mole  $\text{K}^+/\text{L}$

0.30 Mole  $\text{SO}_4^{2-}/\text{L}$

0.01 Mole  $\text{Cl}^-/\text{L}$

0.10 mole  $\text{HCO}_3^-/\text{L}$

Combining all of these constituents to form a single soluble mineral phase, we can define a soluble salt mineral of the form,



In chemical terms, this represents one mole of the soluble salt mineral; if one mole of this mineral were to completely dissolve in one litre of water, it would yield concentrations of dissolved ions as listed above.

In the PHREEQE program the dissolution of this mineral is carried out as the addition of a net stoichiometric reaction, in this case, a mineral dissolution reaction. The starting solution is distilled water to approximate rain water recharge.

Unless the soluble salt mineral is derived from a perfect chemical analysis, there is likely to be some charge imbalance between the total equivalents of anions and cations that make up the mineral. To ensure that the mineral is electrically neutral and, therefore, does not disrupt the electrical neutrality of the solution, it is necessary to add or subtract a quantity of inert negative electrical charge in order to electrically neutralize the soluble mineral. To accomplish this, a quantity of negative charge, corresponding to the amount of imbalance (in equivalents) in the

mineral is added to (in the case of excess cations) or subtracted from (in the case of excess anions) the soluble mineral to ensure neutrality.

The dissolution reaction for the soluble salt, including any charge balancing, is input under the REACTION data block in the PHREEQE program according to the stoichiometry defined by the moles of each constituent in the soluble salt mineral. In general, the dissolution reaction is completed in one step, although it may be done in several steps, if desired.

Evaluating the degree of saturation with respect to calcite, dolomite and gypsum, as minerals of particular interest, is accomplished by examining the LOOK MIN output of the program, and consequently, it is necessary to ensure that at least these three mineral phases are in the LOOK MIN section of the thermodynamic data file. If super-saturation with respect to any of these mineral phases is indicated upon running the spoil mineral dissolution, it is possible to maintain conditions at saturation in subsequent runs by specifying a saturation index value of 0.0 for that mineral(s) under the MINERALS input data block. When this is done, the amount of such mineral(s) precipitated (i.e., the amount in excess of that required for saturation) is included in the output. Ion exchange is also dealt with using MINERALS data block input. The  $K'$  value for the ion exchange reaction is input as the equilibrium constant ( $K_T$ ) with a saturation index equal to 0.00. The partial pressure of  $\text{CO}_2$  is also specified under MINERALS data block input. In this case, the logarithm of the desired  $P_{\text{CO}_2}$  is input as the saturation index, and the value of the equilibrium constant ( $K_T$  @  $25^\circ\text{C}$ ) is equal to the Henry's Law gas constant ( $3.415 \times 10^{-2}$ ).

When a simulation is run, given the series of conditions described above, all of the available salt from the spoil material is allowed to dissolve. Concentrations of species in excess of mineral solubility limits are precipitated and the amount precipitated is calculated. Concentrations of dissolved species are also adjusted to meet the constraints of ion exchange and partial pressure of  $\text{CO}_2$ .

The final resulting solution is at equilibrium with all of the specified mineral phases as well as ion exchange and  $P_{CO_2}$ .

### 3.6.1 Reservoir of Undissolved Salts

In a number of the simulations of spoil groundwater chemistry, the amount of available soluble salt exceeds the solubility limit of several mineral phases, particularly calcite, dolomite, and gypsum. In such cases, the PHREEQE program allows mineral precipitation to occur, maintaining the concentration of dissolved ions at levels corresponding to saturation with respect to the mineral phase. The program also records the amount of mineral precipitation that occurs in terms of moles of mineral per litre of water. Saturation with respect to calcite, dolomite, and gypsum has commonly been observed in spoil groundwater in Alberta (Trudell et al., in press), therefore, the simulated results are consistent with field observations. However, the simulations allow this reservoir of undissolved minerals to be quantified.

Saturation with respect to calcite and dolomite is a ubiquitous feature of both natural and spoil groundwater at the study sites. Not surprisingly then, the simulated spoil groundwater also showed saturation with respect to calcite and dolomite in the majority of cases. However, it is difficult to quantify the amount of carbonate mineral reservoir in the simulated spoil because of the input of bicarbonate to the system from the fixing of the partial pressure of  $CO_2$ . That is, the amount of carbonate mineral precipitated (as calculated by PHREEQE) includes soluble carbonate as determined from the overburden leaching tests, but also includes carbonate derived from the dissolution of  $CO_2$  from the fixed  $P_{CO_2}$ . Consequently, the amount of carbonate precipitated is a function<sup>2</sup> of the soil gas composition in the spoil as well as the salt-yielding properties of the spoil material.

Sulfate is most often precipitated in the form of gypsum, the least soluble of the major sulfate minerals (compared to epsomite and mirabilite, for example). Through the use of PHREEQE to simulate

spoil groundwater chemistry, it is possible to estimate the magnitude of the reservoir of sulfate that remains in the spoil, undissolved, in the form of gypsum. The sulfate precipitated as gypsum is therefore in storage for dissolution by subsequent pore-volumes of fresh groundwater (i.e., a sulfate reservoir). In general, Saturated Paste Extract test data tend to underestimate the magnitude of the sulfate reservoir, probably because gypsum saturation is reached during the test. The 10:1 dilution test, which utilizes a larger water to sediment ratio than the Saturation Extract test, is less likely to encounter gypsum solubility limits and, therefore, provides a better estimate of the total soluble sulfate available in the spoil.

#### 4. EXAMPLE OF PREDICTION OF GROUNDWATER CHEMISTRY

In this section, detailed step-by-step calculations are shown for an example prediction of spoil groundwater chemistry. The starting point for the example is leach-test extract analyses for the two units making up the overburden material (glacial drift and bedrock). These two extract analyses presumably represent some prior grouping of individual samples (e.g., mean and standard deviation or percentile group) by stratigraphic unit as discussed in Section 3.3. The extract results were received as concentrations of dissolved ions in mg/L. Calculations in the example are built from this starting point.

##### 4.1 DETERMINE SALT-YIELD FROM LEACH TEST EXTRACT

For this example a 10:1 water to sediment test is used. The extract analyses and the resultant salt-yield are given in Table 2.

##### 4.2 RELATIVE THICKNESS OF DRIFT AND BEDROCK

Relative thicknesses of the overburden units are calculated to provide its relative proportion in the spoil material.

Table 2. Determination of salt-yield from 10:1 leach tests.

| Constituent                   | Drift Sample |                   | Bedrock Sample |                   |
|-------------------------------|--------------|-------------------|----------------|-------------------|
|                               | mg/L         | g/kg <sup>1</sup> | mg/L           | g/kg <sup>1</sup> |
| Na <sup>+</sup>               | 47.2         | 0.472             | 78.2           | 0.782             |
| K <sup>+</sup>                | 8.1          | 0.081             | 4.2            | 0.042             |
| Ca <sup>2+</sup>              | 8.2          | 0.082             | 4.3            | 0.043             |
| Mg <sup>2+</sup>              | 1.6          | 0.016             | 0.2            | 0.002             |
| SO <sub>4</sub> <sup>2-</sup> | 57.1         | 0.571             | 34.7           | 0.347             |
| HCO <sub>3</sub> <sup>-</sup> | 66.1         | 0.661             | 113.1          | 1.131             |
| Cl <sup>-</sup>               | 5.1          | 0.051             | 5.0            | 0.050             |

<sup>1</sup> g salt per kg spoil calculated using the relationship outlined in Equation (2) (Section 3.2).

From corehole logs,

drift overburden thickness = 3.5 m

Bedrock overburden thickness = 11.2 m

Total overburden thickness = 14.7 m

$$\begin{aligned} \text{Relative thickness of drift} &= \frac{\text{drift thickness}}{\text{total overburden thickness}} \\ &= \frac{3.5 \text{ m}}{14.7 \text{ m}} \\ &= 0.24 \end{aligned}$$

$$\begin{aligned} \text{Relative thickness of bedrock} &= \frac{\text{bedrock overburden thickness}}{\text{total overburden thickness}} \\ &= \frac{11.2 \text{ m}}{14.7 \text{ m}} \\ &= 0.76 \end{aligned}$$

#### 4.3

#### CONSTRUCTING HYPOTHETICAL SPOIL

1. a. The proportion of soluble salt from drift equals the salt-yield from drift multiplied by the proportion of spoil derived from drift (i.e., relative thickness of drift). From the previous section, the relative thickness of drift = 0.24. Table 3 identifies the contribution to the spoil salt-yield from the drift.
- b. The proportion of soluble salt from bedrock equals the salt-yield from bedrock multiplied by the proportion of spoil derived from bedrock (i.e., relative thickness of bedrock). From the previous section, the relative thickness of bedrock = 0.76. Table 4 identifies the contribution of bedrock to the spoil salt-yield.

- c. The salt contribution from the drift and plus bedrock are added to obtain total salt-yield for the hypothetical spoil (Table 5).

Table 3. Determination of drift contribution to spoil salt-yield.

| Constituent                   | Salt-Yield<br>(g/kg) | Contribution to Spoil<br>(g/kg) |
|-------------------------------|----------------------|---------------------------------|
| Na <sup>+</sup>               | 0.472                | 0.1124                          |
| K <sup>+</sup>                | 0.081                | 0.0193                          |
| Ca <sup>2+</sup>              | 0.082                | 0.0195                          |
| Mg <sup>2+</sup>              | 0.016                | 0.0036                          |
| SO <sub>4</sub> <sup>2-</sup> | 0.571                | 0.1360                          |
| HCO <sub>3</sub> <sup>-</sup> | 0.661                | 0.1574                          |
| Cl <sup>-</sup>               | 0.051                | 0.0122                          |

Table 4. Determination of bedrock contribution to spoil salt-yield.

| Constituent                   | Salt-Yield<br>(g/kg) | Contribution to Spoil<br>(g/kg) |
|-------------------------------|----------------------|---------------------------------|
| Na <sup>+</sup>               | 0.782                | 0.7082                          |
| K <sup>+</sup>                | 0.042                | 0.0513                          |
| Ca <sup>2+</sup>              | 0.043                | 0.0523                          |
| Mg <sup>2+</sup>              | 0.002                | 0.0056                          |
| SO <sub>4</sub> <sup>2-</sup> | 0.347                | 0.4004                          |
| HCO <sub>3</sub> <sup>-</sup> | 1.131                | 1.0191                          |
| Cl <sup>-</sup>               | 0.050                | 0.0503                          |

Table 5. Determination of total salt-yield for the hypothetical spoil.

| Constituent                   | Drift Salt Contribution<br>g/kg | Bedrock Salt Contribution<br>g/kg | Total Spoil Salt-Yield<br>g/kg |
|-------------------------------|---------------------------------|-----------------------------------|--------------------------------|
| Na <sup>+</sup>               | 0.1124                          | 0.5958                            | 0.7082                         |
| K <sup>+</sup>                | 0.0193                          | 0.0320                            | 0.0513                         |
| Ca <sup>2+</sup>              | 0.0195                          | 0.0328                            | 0.0523                         |
| Mg <sup>2+</sup>              | 0.0038                          | 0.0018                            | 0.0056                         |
| SO <sub>4</sub> <sup>2-</sup> | 0.1360                          | 0.2644                            | 0.4004                         |
| HCO <sub>3</sub> <sup>-</sup> | 0.1574                          | 0.8617                            | 1.0191                         |
| Cl <sup>-</sup>               | 0.0122                          | 0.0381                            | 0.0503                         |

#### 4.4 SPECIFY BULK DENSITY OF SPOIL AND CALCULATE MASS OF SPOIL IN CONTACT WITH 1 L OF WATER AT SATURATION

The mass of spoil solids ( $M_s$ ) per litre of pore space is calculated using Equation (10) with the following conditions:

$$\rho_s = 2.65 \text{ (g/cm}^3\text{)}$$

$$\rho_b = 1.854 \text{ (g/cm}^3\text{)}$$

$$1.854 \text{ g/cm} = M_s - \left( \frac{1.854 \text{ g/cm}^3}{2.65 \text{ g/cm}^3} \right) M_s$$

$$= M_s - 0.6996 M_s$$

$$0.3004 M_s = 1.854 \text{ g/cm}^3$$

$$M_s = \frac{1.854}{0.3004} \text{ g/cm}^3$$

$$= 6.172 \text{ g/cm}^3$$

$$= 6.172 \text{ kg/L}$$

#### 4.5 CALCULATE THE MOLES OF SALT AVAILABLE TO DISSOLVE IN 1 L OF WATER

From the previous section, there is 6.172 kg of spoil in contact with 1 L of water. Therefore, using Equation (9) the moles of soluble salt in this spoil mass are determined (Table 6).

#### 4.6 SPECIFY GEOCHEMICAL CONDITIONS IN THE SPOIL

1.  $P_{CO_2}$   
From field measurements of spoil gas composition,  $P_{CO_2}$  is estimated to be 0.02 atmospheres,  $\log P_{CO_2} = -1.700$
2. Ca-Na Ion Exchange
  - a. From chemical analyses of groundwater chemistry, determine for each available sample,  $[Ca^{2+}]$  and  $[Na^+]$ . The activity of  $Ca^{2+}$  and  $Na^+$  can be taken from a speciation of the overburden groundwater chemistry using any of a number of geochemical models, such as WATEQF, WATEQ2, PHREEQE, etc.
  - b. For each available chemical analysis of overburden groundwater, calculate a modified selectivity coefficient (Equation (4), Section 3.5.2).

Table 6. Determination of moles of salt available to dissolve in 1L of water.

| Constituent | Gram Formula Weight | Salt-Yield (g/kg) | Moles of Salt/Litre |
|-------------|---------------------|-------------------|---------------------|
| $Na^+$      | 22.991              | 0.7082            | 0.1901              |
| $K^+$       | 39.100              | 0.0513            | 0.0080              |
| $Ca^{2+}$   | 20.040              | 0.0523            | 0.0080              |
| $Mg^{2+}$   | 24.32               | 0.0056            | 0.0014              |
| $SO_4^{2-}$ | 96.066              | 0.4004            | 0.0259              |
| $HCO_3^-$   | 61.019              | 1.0191            | 0.1031              |
| $Cl^-$      | 35.457              | 0.0503            | 0.0086              |

- c. Group the available  $K'$  values according to meaningful stratigraphic units (e.g., drift and bedrock). Calculate a mean and standard deviation for  $K'$  in each group. In this example,  
 for drift,  $\text{mean } K' = 0.00692$ ,  
 $\log \text{mean } K' = -2.160$ ;  
 for bedrock,  $\text{mean } K' = 0.9924$ ,  
 $\log \text{mean } K' = -0.0033$ .
- d. Calculate a thickness-weighted  $K'$  value for the spoil. Using Equation (8), Section 3.5.2, with the relative thickness of drift = 0.2381 and the relative thickness of bedrock = 0.7619  
 $\log K' \text{ spoil} = 0.2381 (\log K' \text{ drift}) + 0.7619$   
 $(\log K' \text{ bedrock})$   
 $= 0.2381 (-2.160) + 0.7619 (-0.0033)$   
 $= -0.5168$
- e. A range of  $K'$  values (min., max.) can be estimated by calculating a spoil  $K'$  as above, using log mean  $\pm 2$  SD values for drift and bedrock.

#### 4.7 APPLICATION OF GEOCHEMICAL MODEL, PHREEQE, TO PRODUCE PREDICTED SPOIL GROUNDWATER CHEMISTRY

The moles of soluble salt available per litre of water (calculated in Section 4.5) are dissolved in 1 L of distilled water under the  $P_{\text{CO}_2}$  and ion exchange conditions specified in Section 4.6 above.

The soluble salt mineral is input under the REACTION data block of PHREEQE, and the  $P_{\text{CO}_2}$  and ion exchange conditions are specified under the MINERALS data block.

The input parameters for PHREEQE to simulate spoil groundwater for the example problem are shown in Figure 5 and given line by line, as follows:

```

1 1  EXAMPLE PHREEQE INPUT DATA FILE FOR PREDICTION OF SPOIL GROUNDWATER CHEM
2 2  004001000 01 8
3 3  SOLUTION 1
4 4  DISTILLED WATER FOR DISSOLUTION OF SOLUBLE MINERAL
5 5  0 0 2 7.00 0. 6.00 1.0
6 6  MINERALS
7 7  FIX PCO2 2 4.00 -1.47 -4.71 0 -1.70
8 8  35 1.00 3 -1.00
9 9  CANAEXCH 2 0.0 -0.5168 0.00 0
10 10  6 2.0 4 -1.0
11 11  CALCITE 2 4.0 -8.47 -2.58 1
12 12  15 1.0 4 1.0
13 13  13.543 -0.0401 -3000.0
14 14  GYPSUM 2 6.0 -4.602 -0.028 0
15 15  16 1.0 4 1.0
16 16
17 17  STEPS
18 18  1.0000
19 19  REACTION
20 20  6 0.1901 0. 7 0.0080 0. 4 0.0080
21 21  16 0.0259 6. 15 0.1030 4. 14 0.0086
22 22  END

```

Figure 5. Example of PHREEQE Input Data File.

Line 1 Title - 80 characters

Line 2

| <u>Parameter</u> | <u>Description</u>                                                                                            | <u>Values Used</u> |
|------------------|---------------------------------------------------------------------------------------------------------------|--------------------|
| IOPT (1)         | Print thermodynamic data<br>= 0 no<br>= 1 yes                                                                 | 0                  |
| IOPT (2)         | = 0, maintain charge imbalance<br>of initial solution                                                         | 0                  |
| IOPT (3)         | = 4, a reaction is added in equal<br>increments                                                               | 4                  |
| IOPT (4)         | = 0, temperature of initial<br>solution is maintained<br>throughout modelling                                 | 0                  |
| IOPT (5)         | = 0, pe constant, same as initial<br>solution                                                                 | 0                  |
| IOPT (6)         | = 0, Debye - Huckel Davies/extended<br>Debye - Huckel equations used<br>to calculate activity<br>coefficients | 0                  |
| IOPT (7)         | = 0, solution composition is not<br>saved for further simulations                                             | 0                  |
| IOPT (8)         | = 0, debugging routine is not called                                                                          | 0                  |
| IOPT (9)         | = 0, no printout of arrays                                                                                    | 0                  |
| NSTEPS           | Number of reaction increments                                                                                 | 1                  |
| NLOMPS           | Number of elements involved in reaction                                                                       | 8                  |
| VO               | Volume of Solution 1 of a titration blank                                                                     | 0                  |
| <u>Line 3</u>    | Data block heading, Solution 1                                                                                |                    |
| <u>Line 4</u>    | Description of Solution 1, in this case,<br>distilled water                                                   |                    |
| <u>Line 5</u>    |                                                                                                               |                    |
| NTOTS            | Number of species in solution                                                                                 | 0                  |
| IALK             | = 0, alkalinity expressed in terms<br>of water                                                                | 0                  |
| IUNITS           | = 2, concentration units mg/L                                                                                 | 2                  |

| <u>Parameter</u> | <u>Description</u>                     | <u>Values Used</u> |
|------------------|----------------------------------------|--------------------|
| PH               | pH                                     | 7.00               |
| PE               | pe                                     | 0.0                |
| TEMP             | Temperature, °C                        | 6.00               |
| SDENS            | Density of solution, g/cm <sup>3</sup> | 1.00               |
| <u>Line 6</u>    | Data block heading, MINERALS           |                    |

The first run of a simulation will usually have only the geochemical conditions specified ( $P_{CO_2}$  and ion exchange). Examination of the 'LOOK MIN' output from the initial run will identify minerals whose solubility limit have been exceeded. These minerals are then included in the 'MINERALS' input block to maintain conditions at saturation. Note that it is not necessary to look up and enter the 'MINERALS' parameters for the minerals phases that are to be held at saturation. The 'LOOK MIN' input data table has the identical parameters in the same format as required for 'MINERALS' input. It is necessary only to copy the desired mineral data from the 'LOOK MIN' table to the appropriate place in the simulation input data file.

#### Lines 7-14

##### First Line

| <u>Parameter</u> | <u>Description</u>                 |
|------------------|------------------------------------|
| MNAME            | Geochemical name                   |
| NMINO            | No. of species                     |
| THMIN            | Total operational valence          |
| LKTOM            | Log equilibrium constant           |
| DHMIN            | Delta $H_r^\circ$ ; kcal/mole      |
| MFLAG            | Van Hoff (0) or analytical (1)     |
| SIMIN            | Saturation index or log $P_{CO_2}$ |

Values Used

|       | Fix $P_{CO_2}$<br>Line 7 <sup>2</sup> | Ca-Na Exchange<br>Lines 9 | Calcite Satn<br>Line 11 | Gypsum<br>Line 14 |
|-------|---------------------------------------|---------------------------|-------------------------|-------------------|
| MNAME | FIX PCO2                              | CANAEXCH                  | CALCITE                 | GYPSUM            |
| NMINO | 2                                     | 2                         | 2                       | 2                 |
| THMIN | 4.00                                  | 0.0                       | 4.0                     | 6.0               |
| LKTOM | -1.47                                 | -0.5168                   | -8.47                   | -4.602            |
| DHMIN | -4.71                                 | 0.0                       | -2.58                   | -0.028            |
| MFLAG | 0                                     | 0                         | 1                       | 0                 |
| SIMIN | -1.70                                 | 0.0                       | 0.0                     | 0.0               |

Second LineParameterDescription

LMIN (1) Index no. of 1st species  
 CMIN (1) Stoichiometric value of 1st species  
 LMIN (2) Index no. of 2nd species  
 CMIN (2) Stoichiometric value of 2nd species

Values Used

|          | Fix $P_{CO_2}$<br>Line 8 <sup>2</sup> | Ca-Na Exchange<br>Lines 10 | Calcite Satn<br>Line 12 | Gypsum<br>Line 15 |
|----------|---------------------------------------|----------------------------|-------------------------|-------------------|
| LMIN (1) | 35                                    | 6                          | 15                      | 16                |
| CMIN (1) | 1.00                                  | 2.00                       | 1.00                    | 1.00              |
| LMIN (2) | 3                                     | 4                          | 4                       | 4                 |
| CMIN (2) | - 1.00                                | -1.00                      | 1.00                    | 1.00              |

Third Line (for calcite saturation, line 13)ParameterDescriptionValue Used

AMIN (1) Analytical constant A1 1.3543E+01  
 AMIN (2) Analytical constant A2 -4.0100E-02  
 AMIN (3) Analytical constant A3 -3.0000E+03  
 AMIN (4) Analytical constant A4 0.0  
 AMIN (5) Analytical constant A5 0.0

Line 16 Blank line, at end of MINERALS data input

Line 17 Data block heading, STEPS

ParameterDescriptionLine 18

XSTEP, increment for reaction, in the example, all of the reaction mineral is dissolved in one increment, therefore XSTEP = 1.00

Line 19

Data block heading REACTION, the soluble salt mineral is input under this data block, which in this example consists of lines 19 and 20.

Line 20

| <u>Constituent</u>            | <u>Parameter</u> | <u>Description</u>                                                          | <u>Values Used</u> |
|-------------------------------|------------------|-----------------------------------------------------------------------------|--------------------|
| Na <sup>+</sup>               | LREAC (1)        | Index number 1st constituent in reaction                                    | 6                  |
|                               | CREAC (1)        | Stoichiometric coefficient (number of moles) of 1st constituent in reaction | 0.190              |
|                               | THMEAN (1)       | Operational valence of 1st constituent                                      | 0.0                |
|                               |                  |                                                                             |                    |
| K <sup>+</sup>                | LREAC (2)        | As above                                                                    | 7                  |
|                               | CREAC (2)        |                                                                             | 0.008              |
|                               | THMEAN (2)       |                                                                             | 0.0                |
| Ca <sup>2+</sup>              | LREAC (3)        |                                                                             | 4                  |
|                               | CREAC (3)        |                                                                             | 0.008              |
|                               | THMEAN (3)       |                                                                             | 0.0                |
| Mg <sup>2+</sup>              | LREAC (4)        |                                                                             | 5                  |
|                               | CREAC (4)        |                                                                             | 0.001              |
|                               | THMEAN (4)       |                                                                             | 0.0                |
| <u>Line 21</u>                |                  |                                                                             |                    |
| SO <sub>4</sub> <sup>2-</sup> | LREAC (5)        |                                                                             | 16                 |
|                               | CREAC (5)        |                                                                             | 0.026              |
|                               | THMEAN (5)       |                                                                             | 6.0                |
| HCO <sub>3</sub> <sup>-</sup> | LREAC (6)        |                                                                             | 15                 |
|                               | CREAC (6)        |                                                                             | 0.1031             |
|                               | THMEAN (6)       |                                                                             | 4.0                |

| <u>Constituent</u>                 | <u>Parameter</u> | <u>Description</u> | <u>Values Used</u> |
|------------------------------------|------------------|--------------------|--------------------|
| Cl <sup>-</sup>                    | LREAC (7)        |                    | 14                 |
|                                    | CREAC (7)        |                    | 0.009              |
|                                    | THMEAN (7)       |                    | 0.0                |
| e <sup>-</sup> (charge<br>balance) | LREAC (8)        |                    | 0.0                |
|                                    | CREAC (8)        |                    | 0.054              |
|                                    | THMEAN (8)       |                    | 0.0                |
| <u>Line 22</u>                     | END              |                    |                    |

The soluble salt 'mineral' from the spoil must be input to REACTION data block as a charge-balanced substance. Since the soluble salt mineral is based on a chemical analysis of leach test extracts, there will always be some analytical imbalance between the total equivalents of cations and anions.

The example soluble salt mineral has an excess of 0.0535 equivalents of cations (Table 7). To accommodate this, PHREEQE can accept the input of 'inert electrical charge', as moles of electrons, to correct the imbalance. This inert charge has index number zero, and is expressed as moles of negative charge to balance the excess of 0.0535 equivalents of positive charge. Note that if the charge

Table 7. Determination of the Charge Balance of the Soluble Salt Mineral.

| <u>Constituent</u>            | <u>Moles</u> | <u>Charge</u> | <u>Equivalents</u> |
|-------------------------------|--------------|---------------|--------------------|
| Na <sup>+</sup>               | 0.1902       | +1            | 0.1902             |
| K <sup>+</sup>                | 0.0080       | +1            | 0.0080             |
| Ca <sup>2+</sup>              | 0.0080       | +2            | 0.0160             |
| Mg <sup>2+</sup>              | 0.0014       | +2            | 0.0028             |
| SO <sub>4</sub> <sup>2-</sup> | 0.0259       | -2            | -0.0518            |
| HCO <sub>3</sub> <sup>-</sup> | 0.1031       | -1            | -0.1031            |
| Cl <sup>-</sup>               | 0.0086       | -1            | -0.0086            |
| Total (charge balance)        |              |               | +0.0535            |

imbalance favored the anions, i.e., excess of negative charge, the corresponding amount of inert electrical charge would be negative. For example, if the charge balance was -0.25 (0.25 equivalents of excess anions), it would be necessary to add -0.25 moles of index number zero (inert negative charge).

Consequently, the soluble salt mineral used in the REACTION data block has eight constituents: seven analytical constituents plus one inert charge constituent.

#### 4.8 INTERPRETATION OF PHREEQE OUTPUT

The output from the model PHREEQE for the example prediction is shown in Figure 6. The output in Figure 6 is annotated to explain the various components of the output.

The final predicted groundwater chemistry appears under the heading 'TOTAL MOLALITIES OF THE ELEMENTS' and 'DESCRIPTION OF SOLUTION' on page 5 of the output (Figure 6). For the example prediction, the final predicted spoil groundwater chemistry is summarized in Table 8.

Table 8. Composition of predicted spoil groundwater.

| Constituent                  | Concentration<br>(Molality = Moles/kg<br>H <sub>2</sub> O) from Printout | Gram<br>Formula<br>Weight               | Concentration<br>mg/L |
|------------------------------|--------------------------------------------------------------------------|-----------------------------------------|-----------------------|
| Na <sup>+</sup>              | 5.34 x 10 <sup>-2</sup>                                                  | 22.991                                  | 1227                  |
| K <sup>+</sup>               | 8.00 x 10 <sup>-3</sup>                                                  | 39.100                                  | 313                   |
| Ca <sup>2+</sup>             | 1.81 x 10 <sup>-2</sup>                                                  | 20.040                                  | 724                   |
| Mg <sup>2+</sup>             | 1.40 x 10 <sup>-4</sup>                                                  | 24.32                                   | 34                    |
| S                            | 1.69 x 10 <sup>-2</sup>                                                  | 96.066 as SO <sub>4</sub> <sup>2-</sup> | 1621                  |
| C                            | 5.06 x 10 <sup>-3</sup>                                                  | 61.019 as HCO <sub>3</sub> <sup>-</sup> | 309                   |
| Cl <sup>-</sup>              | 8.60 x 10 <sup>-3</sup>                                                  | 35.457                                  | 305                   |
| TDS (as sum of constituents) | -                                                                        | -                                       | 4533                  |
| pH                           | -                                                                        | -                                       | 6.92                  |

| DATA ECHO

DATA READ FROM DISK

ELEMENTS  
SPECIES  
LOOK MIN

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 1 of 6).

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 2 of 6).

EXAMPLE PHREEQE INPUT DATA FILE FOR PREDICTION OF SPOIL GROUNDWATER CHEM  
 0040010000 1 8 0.00000  
 SOLUTION 1  
 0 0 2 7.00 0.000E+00 6.00 1.00  
 MINERALS  
 FIX PCO2 2 4.00 -1.47 -4.71 0 -1.700  
 35 1.00 3 -1.00  
 CANAEXCH 2 0.000E+00-0.517 0.000E+00 0 0.000  
 6 2.00 4 -1.00  
 CALCITE 2 4.00 -8.47 -2.58 1 0.000  
 15 1.00 4 1.00  
 1.3543E+01 -4.0100E-02 -3.0000E+03 0.0000E+00 0.0000E+00  
 GYPSUM 2 6.00 -4.60 -0.280E-01 0 0.000  
 16 1.00 4 1.00  
 STEPS 0 0.000E+00 0.000E+00 0.000E+00 0 0.000  
 1.00  
 REACTION  
 6 0.190 0.000 7 0.008 0.000 4 0.008 0.000 \$ 0.001 0.000  
 16 0.026 6.000 15 0.103 4.000 14 0.009 0.000 0 0.054 0.000

ECHO INPUT DATA

```

TOTAL MOLALITIES OF ELEMENTS
-----
ELEMENT      MOLALITY      LOG MOLALITY      CONC MG/L
PURE WATER

-----DESCRIPTION OF SOLUTION-----
PH = 7.0000
PE = 0.0000
ACTIVITY H2O = 1.0000
IONIC STRENGTH = 0.0000
TEMPERATURE = 6.0000
ELECTRICAL BALANCE = 7.8333E-08
TWO = -1.7329E-17
TOTAL ALKALINITY = 2.1695E-08
ITERATIONS = 5
TDS MG/L = 0.0

-----DISTRIBUTION OF SPECIES-----
I  SPECIES  Z      MOLALITY  LOG MOLALITY  ACTIVITY  LOG ACTIVITY  GAMMA      LOG GAMMA
1  H+       1.0      1.00028E-07  -6.9999      1.00000E-07  -7.0000      9.99718E-01  -0.0001
2  E-       -1.0      1.000000E+00  0.0000      1.00000E+00  0.0000      1.00000E+00  0.0000
3  H2O      0.0      1.000000E+00  -0.0000      1.00000E+00  -0.0000      1.00000E+00  0.0000
31 OH-     -1.0      2.16953E-08  -7.6636      2.16952E-08  -7.6638      9.99718E-01  -0.0001
33 H2 AQ   0.0      8.66470E-18  -17.0622     8.66470E-18  -17.0622     1.00000E+00  0.0000

----- LOOK MIN IAP -----
PHASE      LOG IAP      LOG KT      LOG IAP/KT
O2 GAS     -64.8044     -2.8680     -61.9364
H2 GAS     -17.0622     -3.0622     -14.0000

```

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 3 of 6).

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 4 of 6).

STEP NUMBER 1  
-----

1.000E+00 MOLES OF REACTION HAVE BEEN ADDED.

## REACTION IS:

|                  |           |       |
|------------------|-----------|-------|
| 0.19 MOLES OF NA | VALENCE - | 0.000 |
| 0.01 MOLES OF K  | VALENCE - | 0.000 |
| 0.01 MOLES OF CA | VALENCE - | 0.000 |
| 0.00 MOLES OF MG | VALENCE - | 0.000 |
| 0.03 MOLES OF S  | VALENCE - | 6.000 |
| 0.10 MOLES OF C  | VALENCE - | 4.000 |
| 0.01 MOLES OF CL | VALENCE - | 0.000 |
| 0.05 MOLES OF S  | VALENCE - | 0.000 |

ADD SOLUBLE SALT MINERAL

TOTAL MOLALITIES OF ELEMENTS  
-----

| ELEMENT | MOLALITY     | LOG MOLALITY |
|---------|--------------|--------------|
| CA      | 8.000001E-03 | -2.0969      |
| MG      | 1.400000E-03 | -2.8539      |
| NA      | 1.901000E-01 | -0.7210      |
| K       | 8.000001E-03 | -2.0969      |
| CL      | 8.600000E-03 | -2.0655      |
| C       | 1.030000E-01 | -0.9872      |
| S       | 2.590000E-02 | -1.5867      |

CONCENTRATIONS IN SOLUTION BEFORE  
GEOCHEMICAL CONTROLS SPECIFIED BY  
'MINERALS' DATA INPUT BLOCK

## -----PHASE BOUNDARIES-----

| PHASE    | DELTA PHASE*  | LOG IAP | LOG KT  | LOG IAP/KT |
|----------|---------------|---------|---------|------------|
| FIX PCO2 | -4.865316E-02 | -2.9350 | -1.2350 | -1.7000    |
| CANAEXCH | -6.837053E-02 | -0.5168 | -0.5168 | 0.0000     |
| CALCITE  | -4.928278E-02 | -8.3978 | -8.3978 | -0.0000    |
| GYP SUM  | -9.020613E-03 | -4.6006 | -4.6006 | -0.0000    |

GEOCHEMICAL CONTROLS  
- NEGATIVE DELTA PHASE GIVES MOLES OF  
CALCITE (OR OTHER MINERAL PHASES)  
PRECIPITATED PER LITRE OF SPOIL GROUND-  
WATER, 1-e. THE AMOUNT OF PRECIPITATE  
IS THE RE RESERVOIR OF SALT AFTER ONE  
PORE VOLUME OF FLUSHING.

\* NEGATIVE DELTA PHASE INDICATES PRECIPITATION AND POSITIVE DELTA PHASE INDICATES DISSOLUTION.

## ---- LOOK MIN IAP ----

| PHASE    | LOG IAP  | LOG KT   | LOG IAP/KT |
|----------|----------|----------|------------|
| CALCITE  | -8.3978  | -8.3978  | -0.0000    |
| DOLOMITE | -17.8844 | -16.6064 | -1.2780    |
| GYP SUM  | -4.6022  | -4.6006  | -0.0016    |
| PCO2     | -2.9350  | -1.2311  | -1.7039    |
| O2 GAS   | -65.1454 | -2.8680  | -62.2774   |
| H2 GAS   | -16.8925 | -3.0622  | -13.8303   |
| MIRABILI | -5.1252  | -0.1658  | -4.9594    |
| CAOH2    | -17.7449 | -4.7402  | -13.0047   |

LOOK MIN LISTING GIVES SATURATION INDEX  
(IAP/KT) FOR ALL MINERAL PHASES.  
NEGATIVE VALUES ARE UNDERSATURATED;  
POSITIVE ARE SUPERSATURATED; ZERO ARE AT  
SATURATION.

## TOTAL MOLALITIES OF ELEMENTS

| ELEMENT | MOLALITY     | LOG MOLALITY |
|---------|--------------|--------------|
| CA      | 1.806714E-02 | -1.7431      |
| MG      | 1.400000E-03 | -2.8539      |
| NA      | 5.335995E-02 | -1.2728      |
| K       | 8.000001E-03 | -2.0969      |
| CL      | 8.600000E-03 | -2.0655      |
| C       | 5.064046E-03 | -2.2955      |
| S       | 1.667939E-02 | -1.7726      |

CONCENTRATIONS IN SOLUTION AFTER  
APPLICATION OF GEOCHEMICAL CONTROLS.

## ----DESCRIPTION OF SOLUTION----

|                    |   |            |
|--------------------|---|------------|
| PH                 | = | 6.9151     |
| PE                 | = | 0.0000     |
| ACTIVITY H2O       | = | 0.9982     |
| IONIC STRENGTH     | = | 0.0887     |
| TEMPERATURE        | = | 6.0000     |
| ELECTRICAL BALANCE | = | 5.4000E-02 |
| THOR               | = | 1.2153E-01 |
| TOTAL ALKALINITY   | = | 3.9346E-03 |
| ITERATIONS         | = | 24         |

SOLUTION CHARACTERISTICS AFTER  
APPLICATION OF GEOCHEMICAL CONTROLS.-----  
DISTRIBUTION OF SPECIES  
-----

| I  | SPECIES | Z    | MOLALITY    | LOG MOLALITY | ACTIVITY    | LOG ACTIVITY | GAMMA       | LOG GAMMA | NOTE 'GAMMA' IS THE ACTIVITY COEFFICIENT. |
|----|---------|------|-------------|--------------|-------------|--------------|-------------|-----------|-------------------------------------------|
| 1  | H+      | 1.0  | 1.53279E-07 | -6.8145      | 1.21581E-07 | -6.9151      | 7.93205E-01 | -0.1006   |                                           |
| 2  | E-      | -1.0 | 1.00000E+00 | 0.0000       | 1.00000E+00 | 0.0000       | 1.00000E+00 | 0.0000    |                                           |
| 3  | H2O     | 0.0  | 9.98208E-01 | -0.0008      | 9.98208E-01 | -0.0008      | 1.00000E+00 | 0.0000    |                                           |
| 4  | CA+2    | 2.0  | 1.37113E-02 | -1.8629      | 5.67360E-03 | -2.2461      | 4.13790E-01 | -0.3832   |                                           |
| 5  | MG+2    | 2.0  | 1.07815E-03 | -2.9673      | 4.62540E-04 | -3.3349      | 4.29014E-01 | -0.3675   |                                           |
| 6  | NA+     | 1.0  | 5.22747E-02 | -1.2817      | 4.15460E-02 | -1.3815      | 7.94762E-01 | -0.0998   |                                           |
| 7  | K+      | 1.0  | 7.81470E-03 | -2.1071      | 6.08054E-03 | -2.2160      | 7.78142E-01 | -0.1089   |                                           |
| 14 | CL-     | -1.0 | 8.60000E-03 | -2.0655      | 6.69202E-03 | -2.1744      | 7.78142E-01 | -0.1089   |                                           |
| 15 | CO3-2   | -2.0 | 1.72199E-06 | -5.7640      | 7.05182E-07 | -6.1517      | 4.09515E-01 | -0.3877   |                                           |
| 16 | SO4-2   | -2.0 | 1.11417E-02 | -1.9530      | 4.42118E-03 | -2.3545      | 3.96815E-01 | -0.4014   |                                           |
| 31 | OH-     | -1.0 | 2.24498E-08 | -7.6488      | 1.78073E-08 | -7.7494      | 7.93205E-01 | -0.1006   |                                           |
| 33 | H2 AO   | 0.0  | 1.25491E-17 | -16.9014     | 1.28082E-17 | -16.8925     | 1.02064E+00 | 0.0089    |                                           |
| 34 | HCO3-   | -1.0 | 3.71694E-03 | -2.4298      | 2.97340E-03 | -2.5287      | 7.99595E-01 | -0.0969   |                                           |
| 35 | H2CO3   | 0.0  | 1.13585E-03 | -2.9447      | 1.15929E-03 | -2.9358      | 1.02064E+00 | 0.0089    |                                           |
| 40 | HSO4-   | -1.0 | 3.95184E-08 | -7.4032      | 3.13462E-08 | -7.5038      | 7.93205E-01 | -0.1006   |                                           |
| 42 | HS-     | -1.0 | 1.47086E-29 | -28.8324     | 1.16670E-29 | -28.9330     | 7.93205E-01 | -0.1006   |                                           |
| 43 | H2S     | 0.0  | 2.49531E-28 | -27.6029     | 2.54682E-28 | -27.5940     | 1.02064E+00 | 0.0089    |                                           |
| 75 | CAOH+   | 1.0  | 2.79064E-09 | -8.5543      | 2.21355E-09 | -8.6549      | 7.93205E-01 | -0.1006   |                                           |
| 76 | CAC03   | 0.0  | 4.14730E-06 | -5.3822      | 4.23291E-06 | -5.3734      | 1.02064E+00 | 0.0089    |                                           |

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 5 of 6).

Figure 6. Example of PHREEQE Reaction Simulation Output (Page 6 of 6).

|     |         |      |             |         |             |         |             |         |
|-----|---------|------|-------------|---------|-------------|---------|-------------|---------|
| 77  | CAWC03+ | 1.0  | 1.23184E-04 | -3.9094 | 9.77098E-05 | -4.0101 | 7.93205E-01 | -0.1006 |
| 78  | CAS04   | 0.0  | 4.22851E-03 | -2.3738 | 4.31580E-03 | -2.3649 | 1.02064E+00 | 0.0089  |
| 85  | MGOM+   | 1.0  | 1.30866E-09 | -8.8831 | 1.03820E-09 | -8.9837 | 7.93205E-01 | -0.1006 |
| 86  | MEC03   | 0.0  | 2.27809E-07 | -6.6424 | 2.32512E-07 | -6.6336 | 1.02064E+00 | 0.0089  |
| 87  | MHC03+  | 1.0  | 1.82567E-05 | -4.7386 | 1.44813E-05 | -4.8392 | 7.93205E-01 | -0.1006 |
| 88  | ME504   | 0.0  | 3.03368E-04 | -3.5180 | 3.09631E-04 | -3.5092 | 1.02064E+00 | 0.0089  |
| 95  | NAC03-  | -1.0 | 2.45975E-07 | -6.6091 | 1.95109E-07 | -6.7097 | 7.93205E-01 | -0.1006 |
| 96  | NAC03   | 0.0  | 6.34775E-05 | -4.1974 | 6.47879E-05 | -4.1885 | 1.02064E+00 | 0.0089  |
| 97  | NA504-  | -1.0 | 1.02049E-03 | -2.9912 | 8.09455E-04 | -3.0918 | 7.93205E-01 | -0.1006 |
| 100 | KS04-   | -1.0 | 1.85300E-04 | -3.7321 | 1.46981E-04 | -3.8327 | 7.93205E-01 | -0.1006 |

#### 4.9 RESERVOIR OF UNDISSOLVED SALT

From page 4 of 6, of the PHREEQE output (Delta Phase) there are  $4.93 \times 10^{-2}$  moles of calcite precipitated, which represents a reservoir of undissolved salt available for dissolution in subsequent pore volumes of spoil groundwater. As previously discussed (in Section 3.6.1) the reservoir of calcite reflects an input of carbon from the open  $\text{CO}_2$  control, and to some degree, does not necessarily represent the calcite content of the overburden materials or the hypothetical spoil. Also listed under the 'DELTA PHASE' heading on Figure 6, page 4 of 6 of the PHREEQE output,  $9.02 \times 10^{-3}$  moles of gypsum have been precipitated. In this case, the reservoir of undissolved gypsum is an accurate reflection of the spoil after one pore volume of flushing.

The prediction of spoil groundwater chemistry is now complete.

5. REFERENCES

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- Parkhurst, D.L., D.C. Thorstenson, and L.N.P. Plummer. 1980. PHREEQE - a computer program for geochemical calculations. United States Geological Survey, Water Resources Investigations 80-96. NTIS Report Number USGS/WRD/WRI-80/018.
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- Wallick, E.I. 1983. Gas composition in the unsaturated zone as an index of geochemical equilibrium in reclaimed landscapes. In: Proceedings of the Second Alberta Reclamation Conference, Edmonton, Alberta. February 1983. A.W. Fedkenheuer (ed.). Canadian Land Reclamation Association, Publication Number CLRA/AC 83-1. 225-237 pp..

## 6. APPENDICES

- 6.1 SUMMARY DESCRIPTION OF THE USGS GEOCHEMICAL MODEL  
PHREEQE, PARKHURST, THORSTENSON, AND PLUMMER 1980
- PHREEQE stands for pH -redox-equilibrium-equations
  - history - earlier models
    - WATEQ
    - WATEQF
    - SOLMNEQ
    - WATEQ2
  - PHREEQE
    - Computing Information
    - Compiler
      - Fortran H
    - Storage
      - 205K bytes
    - University of Alberta - AMDAHL 470V/7 Computer Execution
      - time usually 1 to 5 sec
  - PHREEQE - capable of dealing with several phases
    - solids
    - liquids
    - gasses
  - can calculate pH and pe
  - mass transfer from one phase to another

### Types of Reactions

1. Adding reactants to a solution.
2. Mixing two waters.
3. Titrating one solution with another.
4. Equilibrating with mineral phases (including multiple phases)
  - a. maintain aqueous phase in equilibrium with mineral phase
  - b. equilibrating with gas
  - c. apparent ion exchange.

Program Calculates

1. pH
2. pE
3. Total concentration of elements.
4. Amount of material transferred into or out of the aqueous phase.
5. Distribution of aqueous species, including ion pairs and complexes.
6. Saturation state with respect to minerals.

6.1.1 Model Structure

## 1. Requirements

- solves  $n$  nonlinear equations in  $n$  unknowns,
- solves four kinds of equations: mass balance for each element; mass action; electron balance; electrical neutrality.

## i. Mass Balance

- must specify the total mass of each element except H and O,
- mass of water assumed to be constant, i.e., 1 kg,

## Mineral Phases

- must keep track of the amount of each element dissolved from or precipitated into solid phase (therefore solubility product of each mineral phase is required),
- must specify the phases present during a reaction.

## ii. Mass Action

- mass action equations, e.g., association reaction for ion pairs, plus equilibrium constant  $K$ ,
- temperature compensation of  $K$  done by using the Van't Hoff, equation (based on enthalpy).

## iii. Redox Reactions

- conservation of electrons,
- bookkeeping technique to keep track of all electrons in the system, (i.e., keep track of oxidation state of the system),
- only applies to species that can be present in reduced or oxidized form, e.g., S, C, Fe; not  $\text{Na}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Cl}^-$ ,
- to keep track, define 'OPERATIONAL VALENCE' (OPV), e.g.,
  1. sulfur:  $\text{SO}_4^{2-}$ :  $\text{OPV} = +6$ ,  $\text{S} = +6$ ,  $\text{O}^2 = 0$  (by convention),
  2.  $\text{CH}_4$ :  $\text{OPV} = 4$ ,  $\text{C} = -4$ ,  $4 \times \text{H} = 0$  (by convention),
  3.  $\text{CO}_2$ :  $\text{OPV} = +4$ ,  $\text{C} = (+4)$ ,  $2 \times \text{O}^2 = 0$ ,
- must define the oxidation state of the solution, i.e., the sum over all species of  $\text{OPV} \times \text{molality}$ ,
- note - can keep track of dissolved  $\text{O}_2$  or  $\text{H}_2$  separately, e.g.,  $\text{H}_2 - \text{OPV} = -2$ ,  $\text{O}_2 - \text{OPV} = +4$ .

## iv. Electrical Neutrality

- pH is calculated based on electrical neutrality of the solution,
- assumes that any charge imbalance in solution is due to analytical error, therefore except for a defined imbalance, solution is charge balanced.

## 2. Master Species

- for each element there are several aqueous species,
- a "MASTER SPECIES" is specified for each element,

- all mass action equations for an element are written in terms of the master species,  
e.g., for Calcium - Master Species  $\text{Ca}^{2+}$ ,  
Sulphur - Master Species  $\text{SO}_4^{2-}$ ,  
Carbon - Master Species  $\text{CO}_3^{2-}$ .

### 3. Thermodynamic Data Base

19 elements (max = 27)

120 aqueous species (max = 250), index 4 to 30 are master species

24 minerals (max = 39)

#### i. Elements

- for each element used in the model, need Name, index member (4 to 30), GFW of species used in analytical data.

#### ii. Species

- name, index number, composition of all aqueous species,
- index 4 to 30 are for master species,
- includes charge of species, OPV, activity coeff. equation info.,
- $\log K_{T0}$  for the association reaction, e.g.,  
 $\text{Ca}^{2+} + \text{CO}_3^{2-} = \text{CaCO}_3$ ,
- H'R for association reaction (kcal/mole),
- all association reactions, K values and H'R values are written using master species, e.g.,  
 $\text{CaHCO}_3^+$ :  $\text{Ca}^{2+} + \text{H}^+ + \text{CO}_3^{2-} = \text{CaHCO}_3^+$ .

#### iii. Look Minerals

- information for minerals for which saturation status is desired,
- format and information is identical to MINERALS input,
- stored in thermodynamic data file,
- not used in any calculations or reactions.

## Summary of PHREEQE Input Data

| Data Block          | Description                                         | Speciation | Type of Simulation            |                    |           |           |
|---------------------|-----------------------------------------------------|------------|-------------------------------|--------------------|-----------|-----------|
|                     |                                                     |            | Equil Sol<br>With<br>Minerals | Mixing<br>2 Waters | Titration | Reaction* |
| 1. Title            |                                                     | U          | U                             | U                  | U         | U         |
| 2. Options          |                                                     | U          | U                             | U                  | U         | U         |
| 3. Elements<br>V    | Thermodynamic<br>Data File                          | U          | U                             | U                  | U         | U         |
| 4. Species<br>V     | Thermodynamic<br>Data File                          | U          | U                             | U                  | U         | U         |
| 5. Solution         | 1 or 2 Initial<br>Solutions                         | U          | U                             | U(1)U(2)           | U(1)U(2)  | U         |
| 6. Minerals         | For Equilibrium<br>With Solution                    | NU         | X                             | X                  | X         | X         |
| 7. Look Min<br>V    | Saturation Status<br>Minerals in Themo<br>Data File | U          | U                             | U                  | U         | U         |
| 8. Temper-<br>ature | If Different<br>From Solution 1                     | NU         | X                             | X                  | X         | X         |
| 9. Steps            | Amount of<br>Reaction Added                         | NU         | NU                            | U                  | U         | U         |
| 10. Reaction        | Define Reaction<br>Added to Solution                | NU         | NU                            | NU                 | NU        | U         |

U - Used

NU - Not used

X - Optional

V - Data stored in thermodynamic data file (Fortran unit 10)

- all other data read on Fortran Unit 5

- output Fortran Unit 6.

\* Simulation of spoil groundwater chemistry procedure corresponds to 'modelling a reaction', where the reaction is the dissolution of salts (from the spoil) into water.

## 6.2

SUMMARY OF PHREEQE INPUT DATA FOR PREDICTION OF SPOIL  
GROUNDWATER CHEMISTRY

Card #1 - Title

Card #2 - Options (IOPT(1) to IOPT(9), NSTEPS, NCOMPS, VO)

- nine options must be specified

| <u>Parameter</u> | <u>Description</u>                                                                                                                                                                                                                                                                                                                                                                                                               | <u>Values Used</u> |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------|
| IOPT (1)         | Print thermodynamic data = 0 no<br>= 1 yes                                                                                                                                                                                                                                                                                                                                                                                       | 0                  |
| IOPT (2)         | Charge balance<br>= 0, maintain charge imbalance of<br>initial sol<br>= 1, adjust pH to obtain charge balance<br>= 2, adjust concentration of one of the<br>elements (e.g., $K^+$ , $Cl^-$ ) to achieve<br>charge balance                                                                                                                                                                                                        | 0                  |
| IOPT (3)         | Reaction modelling option<br>= 0, speciation of solution only; no<br>reactions<br>= 1, mixing of 2 solutions<br>= 2, titration of one solution with<br>another<br>= 3, a reaction is added in specified<br>steps<br>= 4, a reaction is added in equal<br>increments<br>= 5, solution is equilibrated with<br>mineral phases only<br>= 6, reaction is added until equilibrium<br>is reached, with respect to one<br>mineral phase | 4                  |
| IOPT4)           | Temperature option<br>= 0, temperature of initial solution is<br>maintained throughout modelling                                                                                                                                                                                                                                                                                                                                 | 0                  |

| <u>Parameter</u> | <u>Description</u>                                                                                        | <u>Values Used</u> |
|------------------|-----------------------------------------------------------------------------------------------------------|--------------------|
|                  | = 1, temperature constant but different from initial solution                                             |                    |
|                  | = 2, temperature varies in increments during reaction                                                     |                    |
|                  | = 3, temperature of each reaction is specified                                                            |                    |
| IOPT(5)          | Redox option                                                                                              | 0                  |
|                  | = 0, pe constant, same as initial solution                                                                |                    |
|                  | = 1, pe is determined by reaction                                                                         |                    |
| IOPT(6)          | Activity coefficient calculations                                                                         | 0                  |
|                  | = 0, Debye-Huckel/Davies/extended Debye-Huckel equations used depending on available ion size and a' data |                    |
|                  | = 1, Davies formula used except for those specified in thermodynamic data base                            |                    |
| IOPT(7)          | Storage of result solution                                                                                | 0                  |
|                  | = 0, solution composition is not saved for further simulations                                            |                    |
|                  | = 2, save result composition as Solution 2                                                                |                    |
| IOPT(8)          | Debugging - for convergence problems                                                                      | 0                  |
|                  | = 0, debugging print solution is not called                                                               |                    |
|                  | = 1, debugging routine is called                                                                          |                    |
| IOPT(9)          | Array printout - for convergence problems                                                                 | 0                  |
|                  | = 0, no printout of arrays                                                                                |                    |
|                  | = 1, array printed out for each iteration                                                                 |                    |
| NSTEPS           | Number of reaction steps or increments                                                                    | 1                  |
| NCOMPS           | Number of elements involved in a reaction                                                                 | 8                  |
| VO               | Volume of Solution 1 of a titration simulation                                                            |                    |

## Card #3 - Solution description

- i. Solution 1 - starting solution is distilled water
- ii. description
- iii. # of species in solution (NTOTS), for distilled water, NTOTS = 0
  - alkalinity form (IALK) = 0, concentration 0
    - in terms of carbon
    - = 15, concentration terms of alkalinity (e.g.,  $\text{CaCO}_3$ ,  $\text{HCO}_3^-$ ,  $\text{CO}_3^{2-}$ )
  - concentration units (IUNITS) 2
    - = 0 molality
    - = 1 mmol/L
    - = 2 mg/L
    - = 3 ppm
  - pH 7.0
  - pE 0.0
  - temperature °C 6.0
  - density of solution (default = 1.0) 1.0

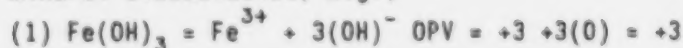
Maintain equilibrium with specified solid and gas phases

- MINERALS input
- two to three cards per mineral
- data and format are identical to the 'LOOK MIN' data base; copy appropriate lines from 'LOOK MIN' to input data file for 'MINERALS' input

Card 1 (a) Mineral name

(b) # species in mineral dissociation

(c) Redox state of mineral - total OPV for the mineral dissociation, e.g.,



- (2)  $\text{CaCO}_3 = \text{Ca}^{2+} + \text{CO}_3^{2-}$  OPV =  $2(0) + 1(+4) = +4$
- (d) Log  $K_{T0}$  Solubility product at 25°C; for gasses,  
 Log  $K_{T0}$  = Henry's law constant, e.g.,  
 for  $\text{CO}_2$  · log  $K_{T0}$  = -1.470
- (e) H'R (kcal/mole) - enthalpy of the reaction
- (f) Temperature dependence  
 FLAG = 0 Van't Hoff equation is used  
 = 1 analytical expression is used
- (g) Saturation index  
 SI = 0 for saturation  
 + ve for supersaturation  
 - ve for undersaturation  
 - for gasses, SI = log of partial pressure of  
 gas, e.g., for 3%  $\text{P}_{\text{CO}_2}$ , log  $\text{P}_{\text{CO}_2}$  = -1.520 = SI

Card 2 Index Number and stoichiometric coeff<sup>2</sup> of each  
 species in the mineral dissolution reaction

Card 3 Analytical expression parameters for temperature  
 dependence of K, if Van't Hoff not used

Card 4 Blank card

#### Modelling Reactions

- three kinds of input data involved
- 1. Temperature (if not constant temp) - generally  
 constant temperature within one run is used, e.g., 6°C
- 2. Steps - defines increments of the reaction process,  
 total # moles of reaction added.
- 3. Reaction - describes stoichiometry and valence of  
 elements added to solution by reaction.

Card 1 STEPS input:

For a reaction added to solution (IOPT(3)=3,4), input  
 # moles of reaction, i.e., STEPS = 1.0; 1.0 mole of  
 spoil 'salt' is being added.

Card 2 - defines the reaction to be added to solution,  
 i.e., moles per litre of each ionic species that makes  
 up the spoil 'salt'

- i. index number of element - index number must be between 4 and 30,
- ii. stoichiometric coefficient of element,
- iii. OPV of the element in the reaction.

---

Finally, END card.

## Reclamation Research Reports

1. **RRTAC 79-2: Proceedings: Workshop on Native Shrubs in Reclamation.** P.F. Ziemkiewicz, C.A. Dermott and H.P. Sims (Editors). 104 pp. No longer available.

The Workshop was organized as the first step in developing a Native Shrub reclamation research program. The Workshop provided a forum for the exchange of information and experiences on three topics: propagation; outplanting; and, species selection. Seven papers and the results of three discussion groups are presented.

2. **RRTAC 80-1: Test Plot Establishment: Native Grasses for Reclamation.** R.S. Sadasivalah and J. Weljer. 19 pp. No longer available.

The report details the species used at three test plots in Alberta's Eastern Slopes (one at Caw Creek Ridge and two at Cadomin). Site preparation, experimental design, and planting method are also described.

3. **RRTAC 80-3: The Role of Organic Compounds in Salinization of Plains Coal Mining Sites.** N.S.C. Cameron et al. 46 pp. \$10.00

This is a literature review of the chemistry of sodic mine spoil and the changes expected to occur in groundwater.

4. **RRTAC 80-4: Proceedings: Workshop on Reconstruction of Forest Soils in Reclamation.** P.F. Ziemkiewicz, S.K. Takyl and H.F. Regler (Editors). 160 pp. \$10.00

Experts in the field of forestry and forest soils report on research relevant to forest soil reconstruction and discuss the most effective means of restoring forestry capability of mined lands.

5. **RRTAC 80-5: Manual of Plant Species Suitability for Reclamation in Alberta.** L.E. Watson, R.W. Parker and D.F. Polster. 2 vols, 541 pp. No longer available.

Forty-three grass, fourteen forb, and thirty-four shrub and tree species are assessed in terms of their suitability for use in reclamation. Range maps, growth habit, propagation, tolerance, and availability information are provided.

6. **RRTAC 81-2: 1980 Survey of Reclamation Activities in Alberta.** D.G. Walker and R.L. Rothwell. 76 pp. \$10.00

This survey is an update of a report prepared in 1976 on reclamation activities in Alberta, and includes research and operational reclamation, locations, personnel, etc.

7. **RRTAC 81-3: Proceedings: Workshop on Coal Ash and Reclamation.** P.F. Ziemkiewicz, R. Stein, R. Leitch and G. Lutwick (Editors). 253 pp. \$10.00

Presents nine technical papers on the chemical, physical, and engineering properties of Alberta fly and bottom ashes, revegetation of ash disposal sites, and use of ash as a soil amendment. Workshop discussions and summaries are also included.

8. **RRTAC 82-1: Land Surface Reclamation: An International Bibliography.** H.P. Sims and C.B. Powter. 2 vols, 292 pp. \$10.00

Literature to 1980 pertinent to reclamation in Alberta is listed in Vol. 1 and is also on the University of Alberta computing system (in a SPIRES database called RECLAIM). Vol. 2 comprises the keyword index and computer access manual.

9. **RRTAC 82-2: A Bibliography of Baseline Studies in Alberta: Soils, Geology, Hydrology and Groundwater.** C.B. Powter and H.P. Sims. 97 pp. \$5.00

This bibliography provides baseline information for persons involved in reclamation research or in the preparation of environmental impact assessments. Materials, up to date as of December 1981, are available in the Alberta Environment Library.

10. **RRTAC 83-1: Soil Reconstruction Design for Reclamation of Oil Sand Tailings.** Monenco Consultants Ltd. 185 pp. No longer available

Volumes of peat and clay required to amend oil sand tailings were estimated based on existing literature. Separate soil prescriptions were made for spruce, jack pine, and herbaceous cover types. The estimates form the basis of field trials.

11. **RRTAC 83-3: Evaluation of Pipeline Reclamation Practices on Agricultural Lands in Alberta.** Hardy Associates (1978) Ltd. 205 pp. No longer available.

Available information on pipeline reclamation practices was reviewed. A field survey was then conducted to determine the effects of pipe size, age, soil type, construction method, etc. on resulting crop production.

12. **RRTAC 83-4: Proceedings: Effects of Coal Mining on Eastern Slopes Hydrology.** P.F. Ziemkiewicz (Editor). 123 pp. \$10.00

Technical papers are presented dealing with the impacts of mining on mountain watersheds, their flow characteristics, and resulting water quality. Mitigative measures and priorities were also discussed.

13. **RRTAC 83-5: Woody Plant Establishment and Management for Oil Sands Mine Reclamation.** Techman Engineering Ltd. 124 pp. No longer available.

This is a review and analysis of information on planting stock quality, rearing techniques, site preparation, planting, and procedures necessary to ensure survival of trees and shrubs in oil sand reclamation.

14. **RRTAC 84-1: Land Surface Reclamation: A Review of the International Literature.** H.P. Sims, C.B. Powter and J.A. Campbell. 2 vols, 1549 pp. \$20.00

Nearly all topics of interest to reclamationists including mining methods, soil amendments, revegetation, propagation and toxic materials are reviewed in light of the international literature.

15. **RRTAC 84-2: Propagation Study: Use of Trees and Shrubs for Oil Sand Reclamation.** Techman Engineering Ltd. 58 pp. \$10.00

This report evaluates and summarizes all available published and unpublished information on large-scale propagation methods for shrubs and trees to be used in oil sand reclamation.

16. **RRTAC 84-3: Reclamation Research Annual Report - 1983.** P.F. Ziemkiewicz. 42 pp. \$5.00

This report details the Reclamation Research Program indicating priorities, descriptions of each research project, researchers, results, and expenditures.

17. **RRTAC 84-4: Soil Microbiology in Land Reclamation.** D. Parkinson, R.M. Danielson, C. Griffiths, S. Visser and J.C. Zak. 2 vols, 676 pp. \$10.00

This is a collection of five reports dealing with re-establishment of fungal decomposers and mycorrhizal symbionts in various amended spoil types.

18. **RRTAC 85-1: Proceedings: Revegetation Methods for Alberta's Mountains and Foothills.**  
P.F. Ziembkiewicz (Editor). 416 pp. \$10.00

Results of long-term experiments and field experience on species selection, fertilization, reforestation, topsoiling, shrub propagation and establishment are presented.

19. **RRTAC 85-2: Reclamation Research Annual Report - 1984.** P.F. Ziembkiewicz. 29 pp. \$5.00

This report details the Reclamation Research Program indicating priorities, descriptions of each research project, researchers, results, and expenditures.

20. **RRTAC 86-1: A Critical Analysis of Settling Pond Design and Alternative Technologies.**  
A. Somanl. 372 pp. \$10.00

The report examines the critical issue of settling pond design, and sizing and alternative technologies. The study was co-funded with The Coal Association of Canada.

21. **RRTAC 86-2: Characterization and Variability of Soil Reconstructed after Surface Mining in Central Alberta.** T.M. Macyk. 146 pp. \$10.00

Reconstructed soils representing different materials handling and replacement techniques were characterized, and variability in chemical and physical properties was assessed. The data obtained indicate that reconstructed soil properties are determined largely by parent material characteristics and further tempered by materials handling procedures. Mining tends to create a relatively homogeneous soil landscape in contrast to the mixture of diverse soils found before mining.

22. **RRTAC 86-3: Generalized Procedures for Assessing Post-Mining Groundwater Supply Potential in the Plains of Alberta - Plains Hydrology and Reclamation Project.**  
M.R. Trudell and S.R. Moran. 30 pp. \$5.00

In the Plains region of Alberta, the surface mining of coal generally occurs in rural, agricultural areas in which domestic water supply requirements are met almost entirely by groundwater. Consequently, an important aspect of the capability of reclaimed lands to satisfy the needs of a residential component is the post-mining availability of groundwater. This report proposes a sequence of steps or procedures to identify and characterize potential post-mining aquifers.

23. **RRTAC 86-4: Geology of the Battle River Site: Plains Hydrology and Reclamation Project.**  
A. Maslowski-Schutze, R. Li, M. Fenton and S.R. Moran. 86 pp. \$10.00

This report summarizes the geological setting of the Battle River study site. It is designed to provide a general understanding of geological conditions adequate to establish a framework for hydrogeological and general reclamation studies. The report is not intended to be a detailed synthesis such as would be required for mine planning purposes.

24. **RRTAC 86-5: Chemical and Mineralogical Properties of Overburden: Plains Hydrology and Reclamation Project.** A. Maslowski-Schutze. 71 pp. \$10.00

This report describes the physical and mineralogical properties of overburden materials in an effort to identify individual beds within the bedrock overburden that might be significantly different in terms of reclamation potential.

25. **RRTAC 86-6: Post-Mining Groundwater Supply at the Battle River Site: Plains Hydrology and Reclamation Project.** M.R. Trudell, G.J. Sterenberg and S.R. Moran. 49 pp. \$5.00

The report deals with the availability of water supply in or beneath cast overburden to support post-mining land use, including both quantity and quality considerations. The study area is in the Battle River Mining area in east-central Alberta.

26. **RRTAC 86-7: Post-Mining Groundwater Supply at the Highvale Site: Plains Hydrology and Reclamation Project.** M.R. Trudell. 25 pp. \$5.00

This report evaluates the availability of water supply in or beneath cast overburden to support post-mining land use, including both quantity and quality considerations. The study area is the Highvale mining area in west-central Alberta.

27. **RRTAC 86-8: Reclamation Research Annual Report - 1985.** P.F. Ziemkiewicz. 54 pp. \$5.00

This report details the Reclamation Research Program indicating priorities, descriptions of each research project, researchers, results, and expenditures.

28. **RRTAC 86-9: Wildlife Habitat Requirements and Reclamation Techniques for the Mountains and Foothills of Alberta.** J.E. Green, R.E. Salter and D.G. Walker. 285 pp. \$10.00

This report presents a review of relevant North American literature on wildlife habitats in mountain and foothills biomes, reclamation techniques, potential problems in wildlife habitat reclamation, and potential habitat assessment methodologies. Four biomes (Alpine, Subalpine, Montane, and Boreal Uplands) and 10 key wildlife species (snowshoe hare, beaver, muskrat, elk, moose, caribou, mountain goat, bighorn sheep, spruce grouse, and white-tailed ptarmigan) are discussed. The study was co-funded with The Coal Association of Canada.

29. **RRTAC 87-1: Disposal of Drilling Wastes.** L.A. Leskiw, E. Reim-Dwyer, T.L. Dabrowski, B.J. Rutherford and H. Hamilton. 210 pp. No longer available.

Current drilling waste disposal practices are reviewed and criteria in Alberta guidelines are assessed. The report also identifies research needs and indicates mitigation measures. A manual provides a decision-making flowchart to assist in selecting methods of environmentally safe waste disposal.

30. **RRTAC 87-2: Minesoil and Landscape Reclamation of the Coal Mines in Alberta's Mountains and Foothills.** A.W. Fedkenheuer, L.J. Knapik and D.G. Walker. 174 pp. \$10.00

This report reviews current reclamation practices with regard to site and soil reconstruction and re-establishment of biological productivity. It also identifies research needs in the Mountain-Foothills area. The study was co-funded with The Coal Association of Canada.

31. **RRTAC 87-3: Gel and Saline Drilling Wastes in Alberta: Workshop Proceedings.** D.A. Lloyd (Compiler). 218 pp. \$10.00

Technical papers were presented which describe: mud systems used and their purpose; industrial constraints; government regulations, procedures and concerns; environmental considerations in waste disposal; and toxic constituents of drilling wastes. Answers to a questionnaire distributed to participants are included in an appendix.

32. **RRTAC 87-4: Reclamation Research Annual Report - 1986.** 50 pp. \$5.00

This report details the Reclamation Research Program indicating priorities, descriptions of each research project, researchers, results, and expenditures.

33. **RRTAC 87-5: Review of the Scientific Basis of Water Quality Criteria for the East Slope Foothills of Alberta.** Beak Associates Consulting Ltd. 46 pp. \$10.00

The report reviews existing Alberta guidelines to assess the quality of water drained from coal mine sites in the East Slope Foothills of Alberta. World literature was reviewed within the context of the East Slopes environment and current mining operations. The ability of coal mine operators to meet the various guidelines is discussed. The study was co-funded with The Coal Association of Canada.

34. **RRTAC 87-6: Assessing Design Flows and Sediment Discharge on the Eastern Slopes.** Hydrocon Engineering (Continental) Ltd. and Monenco Consultants Ltd. 97 pp. \$10.00

The report provides an evaluation of current methodologies used to determine sediment yields due to rainfall events in well-defined areas. Models are available in Alberta to evaluate water and sediment discharge in a post-mining situation. SEDIMOT II (Sedimentology Disturbed Modelling Techniques) is a single storm model that was developed specifically for the design of sediment control structures in watersheds disturbed by surface mining and is well suited to Alberta conditions. The study was co-funded with The Coal Association of Canada.

35. **RRTAC 87-7: The Use of Bottom Ash as an Amendment to Sodic Spoil.** S. Fullerton. 83 pp. No longer available.

The report details the use of bottom ash as an amendment to sodic coal mine spoil. Several rates and methods of application of bottom ash to sodic spoil were tested to determine which was the best at reducing the effects of excess sodium and promoting crop growth. Field trials were set up near the Vesta mine in East Central Alberta using ash readily available from a nearby coal-fired thermal generating station. The research indicated that bottom ash incorporated to a depth of 30 cm using a subsoiler provided the best results.

36. **RRTAC 87-8: Waste Dump Design for Erosion Control.** R.G. Chopluk and S.E. Thornton. 45 pp. \$5.00

This report describes a study to evaluate the potential influence of erosion from reclaimed waste dumps on downslope environments such as streams and rivers. Sites were selected from coal mines in Alberta's mountains and foothills, and included resloped dumps of different configurations and ages, and having different vegetation covers. The study concluded that the average annual amount of surface erosion is minimal. As expected, erosion was greatest on slopes which were newly regraded. Slopes with dense grass cover showed no signs of erosion. Generally, the amount of erosion decreased with time, as a result of initial loss of fine particles, the formation of a weathered surface, and increased vegetative cover.

37. **RRTAC 87-9: Hydrogeology and Groundwater Chemistry of the Battle River Mining Area.** M.R. Trudell, R.L. Faught and S.R. Moran. 97 pp. No longer available.

This report describes the premining geologic conditions in the Battle River coal mining area including the geology as well as the groundwater flow patterns, and the groundwater quality of a sequence of several water-bearing formations extending from the surface to a depth of about 100 metres.

38. **RRTAC 87-10: Soil Survey of the Plains Hydrology and Reclamation Project - Battle River Project Area.** T.M. Macyk and A.H. MacLean. 62 pp. plus 8 maps. \$10.00

The report evaluates the capability of post-mining landscapes and assesses the changes in capability as a result of mining, in the Battle River mining area. Detailed soils information is provided in the report for lands adjacent to areas already mined as well as for lands that are destined to be mined. Characterization of the reconstructed soils in the reclaimed areas is also provided. Data were collected from 1979 to 1985. Eight maps supplement the report.

39. **RRTAC 87-11: Geology of the Highvale Study Site: Plains Hydrology and Reclamation Project.** A. Maslowski-Schutz. 78 pp. \$10.00

The report is one of a series that describes the geology, soils and groundwater conditions at the Highvale Coal Mine study site. The purpose of the study was to establish a summary of site geology to a level of detail necessary to provide a framework for studies of hydrogeology and reclamation.

- 40. RRTAC 87-12: Premining Groundwater Conditions at the Highvale Site. M.R. Trudell and R. Faught. 83 pp. \$10.00**

This report presents a detailed discussion of the premining flow patterns, hydraulic properties, and isotopic and hydrochemical characteristics of five layers within the Paskapoo Geological Formation, the underlying sandstone beds of the Upper Horseshoe Canyon Formation, and the surficial glacial drift.

- 41. RRTAC 87-13: An Agricultural Capability Rating System for Reconstructed Soils. T.M. Macyk. 27 pp. \$5.00**

This report provides the rationale and a system for assessing the agricultural capability of reconstructed soils. Data on the properties of the soils used in this report are provided in RRTAC 86-2.

- 42. RRTAC 88-1: A Proposed Evaluation System for Wildlife Habitat Reclamation in the Mountains and Foothills Biomes of Alberta: Proposed Methodology and Assessment Handbook. T.R. Eccles, R.E. Salter and J.E. Green. 101 pp. plus appendix. \$10.00**

The report focuses on the development of guidelines and procedures for the assessment of reclaimed wildlife habitat in the Mountains and Foothills regions of Alberta. The technical section provides background documentation including a discussion of reclamation planning, a listing of reclamation habitats and associated key wildlife species, conditions required for development, recommended revegetation species, suitable reclamation techniques, a description of the recommended assessment techniques and a glossary of basic terminology. The assessment handbook section contains basic information necessary for evaluating wildlife habitat reclamation, including assessment scoresheets for 15 different reclamation habitats, standard methodologies for measuring habitat variables used as assessment criteria, and minimum requirements for certification. This handbook is intended as a field manual that could potentially be used by site operators and reclamation officers. The study was co-funded with The Coal Association of Canada.

- 43. RRTAC 88-2: Plains Hydrology and Reclamation Project: Spoil Groundwater Chemistry and Its Impacts on Surface Water. M.R. Trudell (Compiler). 135 pp. \$10.00**

Two reports comprise this volume. The first "Chemistry of Groundwater in Mine Spoil, Central Alberta," describes the chemical make-up of spoil groundwater at four mines in the Plains of Alberta. It explains the nature and magnitude of changes in groundwater chemistry following mining and reclamation. The second report, "Impacts of Surface Mining on Chemical Quality of Streams in the Battle River Mining Area," describes the chemical quality of water in streams in the Battle River mining area, and the potential impact of groundwater discharge from surface mines on these streams.

- 44. RRTAC 88-3: Revegetation of Oil Sands Tailings: Growth Improvement of Silver-berry and Buffalo-berry by Inoculation with Mycorrhizal Fungi and N<sub>2</sub>-Fixing Bacteria. S. Visser and R.M. Danielson. 98 pp. \$10.00**

The report provides results of a study: (1) To determine the mycorrhizal affinities of various actinorrhizal shrubs in the Fort McMurray, Alberta region; (2) To establish a basis for justifying symbiont inoculation of buffalo-berry and silver-berry; (3) To develop a growing regime for the greenhouse production of mycorrhizal, nodulated silver-berry and buffalo-berry; and, (4) To conduct a field trial on reconstructed soil on the Syncrude Canada Limited oil sands site to critically evaluate the growth performance of inoculated silver-berry and buffalo-berry as compared with their uninoculated counterparts.

- 45. RRTAC 88-4: Plains Hydrology and Reclamation Project: Investigation of the Settlement Behaviour of Mine Backfill. D.R. Pauls (compiler). 135 pp. \$10.00**

This three part volume covers the laboratory assessment of the potential for subsidence in reclaimed landscapes. The first report in this volume, "Simulation of Mine Spoil Subsidence by Consolidation Tests," covers laboratory simulations of the subsidence process particularly as it is influenced by resaturation of mine spoil. The second report, "Water Sensitivity of Smectitic Overburden: Plains Region of Alberta," describes a series of laboratory tests to determine the behaviour of overburden materials when brought into contact with water. The report entitled "Classification System for Transitional Materials: Plains Region of Alberta," describes a lithological classification system developed to address the characteristics of the smectite rich, clayey transition materials that make up the overburden in the Plains of Alberta.

- 46. RRTAC 88-5: Ectomycorrhizae of Jack Pine and Green Alder: Assessment of the Need for Inoculation, Development of Inoculation Techniques and Outplanting Trials on Oil Sand Tailings. K.M. Danielson and S. Visser. 177 pp. \$10.00**

The overall objective of this research was to characterize the mycorrhizal status of Jack Pine and Green Alder which are prime candidates as reclamation species for oil sand tailings and to determine the potential benefits of mycorrhizae on plant performance. This entailed determining the symbiont status of container-grown nursery stock and the quantity and quality of inoculum in reconstructed soils, developing inoculation techniques and finally, performance testing in an actual reclamation setting.

- 47. RRTAC 88-6: Reclamation Research Annual Report - 1987. Reclamation Research Technical Advisory Committee. 67 pp. No longer available.**

This annual report describes the expenditure of \$500,000.00 of Alberta Heritage Savings Trust Fund monies on research under the Land Reclamation Program. The report outlines the objectives and research strategies of the four program areas, and describes the projects funded under each program.

- 48. RRTAC 88-7: Baseline Growth Performance Levels and Assessment Procedure for Commercial Tree Species in Alberta's Mountains and Foothills. W.R. Dempster and Associates Ltd. 66 pp. \$5.00**

Data on juvenile height development of lodgepole pine and white spruce from cut-over or burned sites in the Eastern Slopes of Alberta were used to define reasonable expectations of early growth performance as a basis for evaluating the success of reforestation following coal mining. Equations were developed predicting total seedling height and current annual height increment as a function of age and elevation. Procedures are described for applying the equations, with further adjustments for drainage class and aspect, to develop local growth performance against these expectations. The study was co-funded with The Coal Association of Canada.

- 49. RRTAC 88-8: Alberta Forest Service Watershed Management Field and Laboratory Methods. A.M.K. Nip and R.A. Hursey. 4 Sections, various pagings. \$10.00**

Disturbances such as coal mines in the Eastern Slopes of Alberta have the potential for affecting watershed quality during and following mining. The collection of hydrometric, water quality and hydrometeorologic information is a complex task. A variety of instruments and measurement methods are required to produce a record of hydrologic inputs and outputs for a watershed basin. There is a growing awareness and recognition that standardization of data acquisition methods is required to ensure data comparability, and to allow comparison of data analyses. The purpose of this manual is to assist those involved in the field of data acquisition by outlining methods, practices and instruments which are reliable and recognized by the International Organization for Standardization.

50. **RRTAC 88-9: Computer Analysis of the Factors Influencing Groundwater Flow and Mass Transport in a System Disturbed by Strip Mining.** F.W. Schwartz and A.S. Crowe. 78 pp. \$10.00

Work presented in this report demonstrates how a groundwater flow model can be used to study a variety of mining-related problems such as declining water levels in areas around the mine as a result of dewatering, and the development of high water tables in spoil once resaturation is complete. This report investigates the role of various hydrogeological parameters that influence the magnitude, timing, and extent of water level changes during and following mining at the regional scale. The modelling approach described here represents a major advance on existing work.

51. **RRTAC 88-10: Review of Literature Related to Clay Liners for Sump Disposal of Drilling Wastes.** D.R. Pauls, S.R. Moran and T. Macyk. 61 pp. \$5.00

The report reviews and analyses the effectiveness of geological containment of drilling waste in sumps. Of particular importance was the determination of changes in properties of clay materials as a result of contact with highly saline brines containing various organic chemicals.

52. **RRTAC 88-11: Highvale Soil Reconstruction Project: Five Year Summary.** D.N. Graveland, T.A. Oddle, A.E. Osborne and L.A. Panek. 104 pp. \$10.00

This report provides details of a five year study to determine a suitable thickness of subsoil to replace over minespoil in the Highvale plains coal mine area to ensure return of agricultural capability. The study also examined the effect of slope and aspect on agricultural capability. This study was funded and managed with industry assistance.

53. **RRTAC 88-12: A Review of the International Literature on Mine Spoil Subsidence.** J.D. Scott, G. Zinter, D.R. Pauls and M.B. Dusseault. 36 pp. \$10.00

The report reviews available engineering literature relative to subsidence of reclaimed mine spoil. The report covers methods for site investigation, field monitoring programs and lab programs, mechanisms of settlement, and remedial measures.

54. **RRTAC 89-1: Reclamation Research Annual Report - 1988.** 74 pp. \$5.00

This annual report describes the expenditure of \$280,000.00 of Alberta Heritage Savings Trust Fund monies on research under the Land Reclamation Program. The report outlines the objectives and research strategies of the four program areas, and describes the projects funded under each program.

55. **RRTAC 89-2: Proceedings of the Conference: Reclamation, A Global Perspective.** D.G. Walker, C.B. Powter and M.W. Pole (Compilers). 2 Vols., 854 pp. \$10.00

Over 250 delegates from all over the world attended this conference held in Calgary in August, 1989. The proceedings contains over 85 peer-reviewed papers under the following headings: A Global Perspective; Northern and High Altitude Reclamation; Fish & Wildlife and Rangeland Reclamation; Water; Herbaceous Revegetation; Woody Plant Revegetation and Succession; Industrial and Urban Sites; Problems and Solutions; Sodic and Saline Materials; Soils and Overburden; Acid Generating Materials; and, Mine Tailings.

56. **RRTAC 89-3: Efficiency of Activated Charcoal for Inactivation of Bromacil and Tebuthiuron Residues in Soil.** M.P. Sharma. 38 pp. \$5.00

Bromacil and Tebuthiuron were commonly used soil sterilants on well sites, battery sites and other industrial sites in Alberta where total vegetation control was desired. Activated charcoal was found to be effective in binding the sterilants in greenhouse trials. The influence of factors such as herbicide:charcoal concentration ratio, soil texture, organic matter content, soil moisture, and the time interval between charcoal incorporation and plant establishment were evaluated in the greenhouse.

- 57. RRTAC 89-4: Manual of Plant Species Suitability for Reclamation in Alberta - 2nd Edition. Hardy BBT Limited. 436 pp. \$10.00**

This is an updated version of RRTAC Report 80-5 which describes the characteristics of 43 grass, 14 forb and 34 shrub and tree species which make them suitable for reclamation in Alberta. The report has been updated in several important ways: a line drawing of each species has been added; the range maps for each species have been redrawn based on an ecosystem classification of the province; new information (to 1990) has been added, particularly in the sections on reclamation use; and the material has been reorganized to facilitate information retrieval. Of greatest interest is the performance chart that precedes each species and the combined performance charts for the grass, forb, and shrub/tree groups. These allow the reader to pick out at a glance species that may suit their particular needs. The report was produced with the assistance of a grant from the Recreation, Parks and Wildlife Foundation.

- 58. RRTAC 89-5: Battle River Soil Reconstruction Project Five Year Summary. L.A. Leskiw. 188 pp. \$10.00**

This report summarizes the results of a five year study to investigate methods required to return capability to land surface mined for coal in the Battle River area of central Alberta. Studies were conducted on: the amounts of subsoil required, the potential of gypsum and bottom ash to amend adverse soil properties, and the effects of slope angle and aspect. Forage and cereal crop growth was evaluated, as were changes in soil chemistry, density and moisture holding characteristics.

- 59. RRTAC 89-6: Detailed Sampling, Characterization and Greenhouse Pot Trials Relative to Drilling Wastes in Alberta. T.M. Macyk, F.I. Nikiforuk, S.A. Abboud and Z.W. Widtman. 228 pp. \$10.00**

This report summarizes a three-year study of the chemistry of freshwater gel, KCl, NaCl, DAP, and invert drilling wastes, both solids and liquids, from three regions in Alberta: Cold Lake, Eastern Slopes, and Peace River/Grande Prairie. A greenhouse study also examined the effects of adding various amounts of waste to soil on grass growth and soil chemistry. Methods for sampling drilling wastes are recommended.